

-1-

CAR LIGAND-BINDING DOMAIN POLYPEPTIDE CO-CRYSTALLIZED WITH
A LIGAND, AND METHODS OF DESIGNING LIGANDS THAT MODULATE
CAR ACTIVITY

5

Technical Field

The present invention relates generally to the structure of the ligand-binding domain of CAR, and more particularly to the structure of the ligand-binding domain of CAR in complex with a ligand. The present invention also relates to CAR binding compounds and to the design of compounds that bind to CAR.

10

Abbreviations

	amu	-	atomic mass unit(s)
	ATP	-	adenosine triphosphate
15	ADP	-	adenosine diphosphate
	BSA	-	bovine serum albumin
	CaMV	-	cauliflower mosaic virus
	CAR	-	constitutive androstane receptor
	CAR α	-	constitutive androstane receptor alpha
20	CBP	-	CREB binding protein
	CCDB	-	Cambridge Crystallographic Data Bank
	cDNA	-	complementary DNA
	CPU	-	central processing unit
	RAM	-	random access memory
25	CRT	-	cathode-ray tube
	DBD	-	DNA binding domain
	DMSO	-	dimethyl sulfoxide
	DNA	-	deoxyribonucleic acid
	DTT	-	dithiothreitol
30	EDTA	-	ethylenediaminetetraacetic acid
	Et ₂ O	-	diethyl ether
	FEDs	-	field emission displays

-2-

	GST	-	glutathione S-transferase
	HEPES	-	N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic acid
	kDa	-	kilodalton(s)
5	LBD	-	ligand-binding domain
	LCDs	-	liquid crystal displays
	LED	-	light emitting diode
	MPD	-	methyl-pentenediol
	MCAR	-	mouse constitutive androstane receptor
10	MIR	-	multiple isomorphous replacement
	MPD	-	methyl pentenediol
	N-COR	-	nuclear co-repressor
	NDP	-	nucleotide diphosphate
	NR	-	nuclear receptor
15	nt	-	nucleotide(s)
	NTP	-	nucleotide triphosphate
	PAGE	-	polyacrylamide gel electrophoresis
	PCR	-	polymerase chain reaction
	PEG	-	polyethylene glycol
20	pl	-	isoelectric point
	PXR	-	pregnane X receptor
	PBREM	-	phenobarbital-responsive enhancer module
	RAR	-	retinoic acid receptor
	RAREs	-	retinoic acid response elements
25	rCAR	-	rat constitutive androstane receptor
	RUBISCO	-	ribulose biphosphate carboxylase
	RXR	-	retinoid X receptor
	SDS	-	sodium dodecyl sulfate
30	SDS-PAGE	-	sodium dodecyl sulfate polyacrylamide gel electrophoresis
	SMRT	-	silencing mediator for retinoid and thyroid receptors

-3-

5	SRC-1	-	steroid receptor coactivator-1
	SR	-	steroid receptor
	TFA	-	trifluoroacetic acid
	TMV	-	tobacco mosaic virus
	TR	-	thyroid receptor
	VDR	-	vitamin D receptor

Amino Acid Abbreviations, Codes, and Functionally Equivalent Codons

	<u>Amino Acid</u>	<u>3-Letter</u>	<u>1-Letter</u>	<u>Codons</u>
10	Alanine	Ala	A	GCA GCC GCG GCU
	Arginine	Arg	R	AGA AGG CGA CGC CGG CGU
	Asparagine	Asn	N	AAC AAU
	Aspartic Acid	Asp	D	GAC GAU
	Cysteine	Cys	C	UGC UGU
15	Glutamic acid	Glu	E	GAA GAG
	Glutamine	Gln	Q	CAA CAG
	Glycine	Gly	G	GGA GGC GGG GGU
	Histidine	His	H	CAC CAU
	Isoleucine	Ile	I	AUA AUC AUU
20	Leucine	Leu	L	UUA UUG CUA CUC CUG CUU
	Lysine	Lys	K	AAA AAG
	Methionine	Met	M	AUG
	Phenylalanine	Phe	F	UUC UUU
	Proline	Pro	P	CCA CCC CCG CCU
25	Serine	Ser	S	ACG AGU UCA UCC UCG UCU
	Threonine	Thr	T	ACA ACC ACG ACU
	Tryptophan	Trp	W	UGG
	Tyrosine	Tyr	Y	UAC UAU
	Valine	Val	V	GUA GUC GUG GUU

30

-4-

Background

The constitutive androstane receptor (CAR; Unified Nomenclature Committee designation NR1I3) was isolated in 1994 by screening a human liver library with a degenerate oligonucleotide probe based on the P box region (Baes *et al.*, 1994). CAR was subsequently shown to be a heterodimer partner for RXR that acts as a specific, retinoid-independent activator of a subset of retinoic acid response elements (RAREs). The mouse CAR homologue was also isolated in 1994 (Honkakoski *et al.*, 1998). Mouse CAR studies showed that RXR and CAR bind to a site in the phenobarbital-responsive enhancer module (PBREM) of the cytochrome P-450 *Cyp2b10* gene in response to phenobarbital induction. Expression of RXR and CAR in mammalian cell lines activated PBREM, indicating that a CAR-RXR heterodimer is a trans-acting factor for the mouse *Cyp2b10* gene. These studies were the first to indicate that CAR might play a role in response to xenobiotics.

The ability to respond to a wide range of potentially toxic chemicals is essential in a complex environment. Evidence is accumulating that CAR and its closest mammalian homologue, the pregnane X receptor (PXR; Unified Nomenclature Committee designation NR1I2), evolved to detect xenobiotics as part of the body's detoxification machinery (Waxman, 1999). Both receptors are highly expressed in the liver and intestine and both regulate the expression of specific detoxification genes. PXR and CAR regulate genes whose protein products are involved in the hydroxylation (phase I), conjugation (phase II), and transport of xenobiotics (phase III). CAR is activated by some of the same ligands as PXR (Moore *et al.*, 2000), regulates at least partially overlapping sets of genes (*e.g. CYP3A and CYP2B*; Xie *et al.*, 2000a), and can signal through the same response elements (Goodwin *et al.*, 2001; Handschin *et al.*, 2001).

Despite these similarities, CAR differs from PXR in several respects. CAR ligand binding has been shown to be more restricted than that of PXR (Moore *et al.*, 2000). Furthermore, CAR displays a high basal level of activity relative to PXR that can be reduced by the binding of either naturally

-5-

occurring androstanes or xenobiotics such as clotrimazole (Baes *et al.*, 1994; Moore *et al.*, 2000). Finally, CAR displays fundamental differences from PXR with regard to its cellular regulation. In mouse primary hepatocytes and in mouse liver *in vivo*, CAR is cytoplasmic in the naïve state and translocates to the nucleus upon activation (Kawamoto *et al.*, 1999), a process thought to be regulated in part by dephosphorylation of the receptor (Honkakoski *et al.*, 1998). Induction of CAR nuclear translocation does not necessarily depend upon ligand-binding, as phenobarbital has been shown to be an activator of CAR *in vivo* and in hepatocytes, but does not appear to interact directly with the CAR ligand-binding domain (Moore *et al.*, 2000). Thus, CAR has a high basal level of transcriptional activity even in the absence of an exogenous ligand. An important goal of future efforts will be to further differentiate the physical and functional properties of CAR from PXR, and to ultimately distinguish the unique physiological role of CAR.

Towards this goal, the CAR gene has recently been "knocked-out" by targeted gene disruption (Xie *et al.*, 2000b). The loss of CAR expression did not result in any overt phenotype. Homozygous CAR^{-/-} animals were born at the expected Mendelian frequency, and both male and female CAR-deficient animals were fertile. It was further demonstrated that the nuclear receptor CAR mediates the Cyp2b10 gene response evoked by phenobarbital-like inducers, as well as by the more potent TCPOBOP compound (Xie *et al.*, 2000b). When challenged, these animals showed decreased metabolism of the classic CYP substrate zoxazolamine and a complete loss of the liver hypertrophic and hyperplastic responses to these compounds. These experiments were thus consistent with the notion that at least one aspect of the physiological role of CAR involves xenobiotic metabolism.

Further insight into CAR is expected to be gleaned from CAR structural studies. The availability of the CAR structure will allow an understanding of ligand modulation of CAR activity and will facilitate the design of novel CAR ligands. The present invention addresses these and other needs in the art.

-6-

Summary of the Invention

The present invention provides a crystalline form comprising a substantially pure constitutive androstane receptor (CAR) ligand-binding domain polypeptide. In one embodiment, the crystalline form comprises a substantially pure constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand. In one embodiment, a ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of generating a crystalline form comprising a constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand, the method comprising: (a) incubating a solution comprising a constitutive androstane receptor (CAR) ligand-binding domain and a ligand with an equal volume of reservoir; and (b) crystallizing the constitutive androstane receptor (CAR) ligand-binding domain polypeptide and ligand using the hanging drop method, whereby a crystalline form of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand is generated. Also provided is a crystalline form formed by the above-recited method. In one embodiment, a ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of designing a chemical compound that modulates the biological activity of a target constitutive androstane receptor (CAR) polypeptide. In one embodiment, the method comprises: obtaining one or more three-dimensional structures for the ligand-binding domain (LBD) of constitutive androstane receptor (CAR) in a repressed conformation, and one or more three-dimensional structures of the LBD of constitutive androstane receptor (CAR) in an activated conformation; rotating and translating the three-dimensional structures as rigid bodies so as to superimpose corresponding backbone atoms of a core region of the constitutive androstane receptor (CAR) LBD; comparing one or both of: (i) the superimposed three-dimensional structures to identify volume near the ligand-binding pocket of the constitutive androstane receptor (CAR) LBD that is available to a ligand in the one or more activated structures, or in one or more

-7-

repressed structures, but that is not available to the ligand in one or more structures of the opposite class; and (ii) the superimposed three-dimensional structures to identify interactions that a ligand could make in one or more of the activated structures, or in one or more of the repressed structures, but
5 which the ligand could not make in one or more structures of the opposite class; and designing a chemical compound that occupies the volume, makes the interaction, or both occupies the volume and makes the interaction.

Optionally the method further comprises synthesizing the designed chemical compound; and testing the designed chemical compound in a
10 biological assay to determine whether it acts as a ligand of constitutive androstane receptor (CAR) with an effect on constitutive androstane receptor (CAR) biological activities, whereby a ligand of a constitutive androstane receptor (CAR) polypeptide is designed.

In another embodiment, the volume or interaction is available in one or
15 more of the repressed structures of constitutive androstane receptor (CAR), but not available in one or more of the activated structures of constitutive androstane receptor (CAR). In another embodiment, the method further comprises designing a chemical compound that promotes the binding of co-repressor to the constitutive androstane receptor (CAR) LBD by making direct
20 favorable interactions with the co-repressor. In another embodiment, the method further comprises designing a chemical compound that reduces binding of a co-repressor to the constitutive androstane receptor (CAR) LBD by making direct unfavorable interactions with the co-repressor. In another embodiment, the method further comprises designing a chemical compound
25 that promotes coactivator binding by displacing an AF2 helix of the constitutive androstane receptor (CAR) LBD and making direct favorable interactions with a coactivator, where the designing allows for an expected movement of the coactivator within a coactivator/co-repressor binding pocket. In yet another embodiment, the method further comprises designing a
30 chemical compound by considering a known agonist of the constitutive androstane receptor (CAR) and adding a substituent that protrudes into the volume identified in step (c) or that makes a desired interaction.

-8-

The present invention also provides a binding site in a human constitutive androstane receptor (CAR) polypeptide for a constitutive androstane receptor ligand, wherein the ligand is in van der Waals, hydrogen binding, or van der Waals and hydrogen binding contact with at least one
5 residue of the human constitutive androstane receptor polypeptide.

The present invention also provides a complex of a human constitutive androstane receptor (CAR) ligand-binding domain and a ligand, wherein the ligand is in van der Waals, hydrogen bonding, or both van der Waals and hydrogen bonding contact with at least one of the following residues of the
10 human constitutive androstane receptor polypeptide: Phe161, Ile164, Asn165, Val199, His203, Phe217, Trp224, Thr225, Ile226, Asp228, Gly229, Gln234, Phe238, Leu239, Leu242, Phe243, Tyr326, Met339, Met340.

The present invention also provides a crystal of a complex of a human constitutive androstane receptor (CAR) ligand-binding domain and a ligand,
15 wherein the ligand is in van der Waals, hydrogen bonding, or both van der Waals and hydrogen bonding contact with at least one of the following residues of the human constitutive androstane receptor polypeptide: Phe161, Ile164, Asn165, Val199, His203, Phe217, Trp224, Thr225, Ile226, Asp228, Gly229, Gln234, Phe238, Leu239, Leu242, Phe243, Tyr326, Met339, Met340.
20 In one embodiment, the constitutive androstane receptor is a human constitutive androstane receptor and the crystal has the following physical measurements: space group $P2_12_12_1$, and unit cell: $a = 83.0$ angstroms, $b = 116.8$ angstroms, $c = 131.9$ angstroms, and $\alpha = \beta = \gamma = 90$ degrees.

The present invention also provides a method for designing a ligand of
25 a constitutive androstane receptor (CAR) polypeptide, the method comprising:
(a) forming a complex of a compound bound to the constitutive androstane receptor (CAR) polypeptide; (b) determining a structural feature of the complex formed in (a); wherein the structural feature is of a binding site for the compound; and (c) using the structural feature determined in (b) to design a
30 ligand of a constitutive androstane receptor (CAR) polypeptide capable of binding to the binding site of the present invention. In one embodiment, the

-9-

method of the present invention further comprises using a computer-based model of the complex formed in (a) in designing the ligand.

The present invention also provides a method of designing a ligand that selectively modulates the activity of a constitutive androstane receptor (CAR) polypeptide, the method comprising: (a) evaluating a three-dimensional structure of a crystallized constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand; and (b) synthesizing a potential ligand based on the three-dimensional structure of the crystallized constitutive androstane receptor (CAR) catalytic polypeptide in complex with a ligand, whereby a ligand that selectively modulates the activity of a constitutive androstane receptor (CAR) polypeptide is designed. In one embodiment, the constitutive androstane receptor (CAR) ligand-binding domain polypeptide comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the crystalline form is such that the three-dimensional structure of the crystallized constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand can be determined to a resolution of about 2.15 Å or better. In one embodiment, the method further comprises contacting a constitutive androstane receptor (CAR) ligand-binding domain polypeptide with the potential ligand and a ligand; and assaying the constitutive androstane receptor (CAR) ligand-binding domain polypeptide for binding of the potential ligand, for a change in activity of the constitutive androstane receptor (CAR) ligand-binding domain polypeptide, or both. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of screening a plurality of compounds for a ligand of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide, the method comprising: (a) providing a library of test samples; (b) contacting a crystalline form comprising a constitutive androstane receptor (CAR) polypeptide in complex with a ligand with each test sample; (c) detecting an interaction between a test sample and the crystalline constitutive androstane receptor (CAR) polypeptide in complex with a ligand; (d) identifying a test sample that interacts with the crystalline

-10-

constitutive androstane receptor (CAR) polypeptide in complex with a ligand; and (e) isolating a test sample that interacts with the crystalline constitutive androstane receptor (CAR) polypeptide in complex with a ligand, whereby a plurality of compounds is screened for a ligand of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide. In one embodiment, the CAR polypeptide comprises a CAR ligand-binding domain. In another embodiment, the CAR polypeptide is a human CAR polypeptide. In yet another embodiment, the CAR polypeptide comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the library of test samples is bound to a substrate. In another embodiment, the library of test samples is synthesized directly on a substrate. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide,

The present invention also provides a method for identifying a constitutive androstane receptor (CAR) ligand, the method comprising: (a) providing atomic coordinates of a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand to a computerized modeling system; and (b) modeling a ligand that fits spatially into the binding pocket of the constitutive androstane receptor (CAR) ligand-binding domain to thereby identify a constitutive androstane receptor (CAR) ligand. In one embodiment, the method further comprises identifying in an assay for constitutive androstane receptor (CAR)-mediated activity a modeled ligand that increases or decreases the activity of the constitutive androstane receptor (CAR). In one embodiment, the CAR is a human CAR. In one embodiment, the CAR ligand-binding domain comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of identifying a constitutive androstane receptor (CAR) ligand that selectively binds a constitutive androstane receptor (CAR) polypeptide compared to other polypeptides, the method comprising: (a) providing atomic coordinates of a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand to a computerized modeling system; and (b) modeling a ligand that

-11-

fits into the binding pocket of a constitutive androstane receptor (CAR) ligand-binding domain and that interacts with residues of a constitutive androstane receptor (CAR) ligand-binding domain that are conserved among constitutive androstane receptor (CAR) subtypes to thereby identify a constitutive androstane receptor (CAR) ligand that selectively binds a constitutive androstane receptor (CAR) polypeptide compared to other polypeptides. In one embodiment, the method further comprises identifying in a biological assay for constitutive androstane receptor (CAR) activity a modeled ligand that selectively binds to said constitutive androstane receptor (CAR) and increases or decreases the activity of the constitutive androstane receptor (CAR). In one embodiment, the CAR ligand-binding domain comprises the amino acid sequence shown in SEQ ID NO: 4. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of designing a ligand of a constitutive androstane receptor (CAR) polypeptide, the method comprising: (a) selecting a candidate constitutive androstane receptor (CAR) ligand; (b) determining which amino acid or amino acids of a constitutive androstane receptor (CAR) polypeptide interact with the ligand using a three-dimensional model of a crystallized protein, the model comprising a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand; (c) identifying in a biological assay for constitutive androstane receptor (CAR) activity a degree to which the ligand modulates the activity of the constitutive androstane receptor (CAR) polypeptide; (d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the constitutive androstane receptor (CAR) polypeptide and the ligand is predicted to be modulated by the chemical modification; (e) synthesizing a ligand having the chemical modified to form a modified ligand; (f) contacting the modified ligand with the constitutive androstane receptor (CAR) polypeptide; (g) identifying in a biological assay for constitutive androstane receptor (CAR) activity a degree to which the modified ligand modulates the biological activity of the constitutive androstane receptor (CAR) polypeptide; and (h) comparing the biological activity of the constitutive androstane

-12-

receptor (CAR) polypeptide in the presence of modified ligand with the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the unmodified ligand, whereby a ligand of a constitutive androstane receptor (CAR) polypeptide is designed. In one embodiment, wherein the method further comprises repeating steps (a) through (f), if the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the modified ligand varies from the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the unmodified ligand.

The present invention also provides a crystallized, recombinant polypeptide comprising: (a) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (b) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (c) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of constitutive androstane receptor (CAR); wherein the polypeptide of (a), (b) or (c) is in crystal form. In one embodiment, the crystallized, recombinant polypeptide diffracts X-rays to a resolution of about 2.5 Å or better. In another embodiment, the polypeptide comprises at least one heavy atom label. In another embodiment, the polypeptide is labeled with seleno-methionine.

The present invention also provides a method for designing a modulator for the prevention or treatment of a disease or disorder, comprising: (a) providing a three-dimensional structure for a crystallized, recombinant polypeptide; (b) identifying a potential modulator for the prevention or treatment of a disease or disorder by reference to the three-dimensional structure; (c) contacting a polypeptide or a constitutive androstane receptor (CAR) with the potential modulator; and (d) assaying the activity of the polypeptide after contact with the modulator, wherein a change in the activity of the polypeptide indicates that the modulator can be useful for prevention or treatment of a disease or disorder.

-13-

The present invention also provides a method for obtaining structural information of a crystallized polypeptide, the method comprising: (a) crystallizing a recombinant polypeptide, wherein the polypeptide comprises: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); and wherein the crystallized polypeptide is capable of diffracting X-rays to a resolution of 2.5 Å or better; and (b) analyzing the crystallized polypeptide by X-ray diffraction to determine the three-dimensional structure of at least a portion of the crystallized polypeptide. In one embodiment, the three-dimensional structure of the portion of the crystallized polypeptide is determined to a resolution of 2.5 Å or better.

The present invention also provides a method for identifying a druggable region of a polypeptide, the method comprising: (a) obtaining crystals of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR), such that the three dimensional structure of the crystallized polypeptide can be determined to a resolution of 2.5 Å or better; (b) determining the three dimensional structure of the crystallized polypeptide using X-ray diffraction; and (c) identifying a druggable region of the crystallized polypeptide based on the three-dimensional structure of the crystallized polypeptide. In one embodiment, the druggable region is an active site. In another embodiment, the druggable region is on the surface of the polypeptide.

-14-

The present invention also provides a crystalline human constitutive androstane receptor (CAR) comprising a crystal having unit cell dimensions $a = 83.0 \text{ \AA}$; $b = 116.8 \text{ \AA}$; $c = 131.9 \text{ \AA}$; $\alpha = \beta = \gamma = 90^\circ$; with an orthorhombic space group $P2_12_12_1$ and 4 molecules per asymmetric unit.

5 The present invention also provides a crystallized polypeptide comprising: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under
10 stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); wherein the crystal has a $P2_12_12_1$ space group.

15 The present invention also provides a crystallized polypeptide comprising a structure of a polypeptide that is defined by a substantial portion of the atomic coordinates set forth in Table 2 or Table 3.

20 The present invention also provides a method for determining the crystal structure of a homolog of a polypeptide, the method comprising: (a) providing the three dimensional structure of a first crystallized polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under
25 stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) obtaining crystals of a second polypeptide comprising an amino acid sequence that is at least 70% identical to the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4, such that the three dimensional structure of the second crystallized
30 polypeptide can be determined to a resolution of 2.5 \AA or better; and (c) determining the three dimensional structure of the second crystallized polypeptide by X-ray crystallography based on the atomic coordinates of the

-15-

three dimensional structure provided in step (a). In one embodiment, the atomic coordinates for the second crystallized polypeptide have a root mean square deviation from the backbone atoms of the first polypeptide of not more than 1.5 Å for all backbone atoms shared in common with the first polypeptide and the second polypeptide.

The present invention also provides a method for homology modeling a homolog of human constitutive androstane receptor (CAR), comprising: (a) aligning the amino acid sequence of a homolog of human constitutive androstane receptor (CAR) with an amino acid sequence of SEQ ID NO: 2 or SEQ ID NO: 4 and incorporating the sequence of the homolog of human CAR into a model of human constitutive androstane receptor (CAR) derived from structure coordinates as listed in Table 2 or Table 3 to yield a preliminary model of the homolog of human CAR; (b) subjecting the preliminary model to energy minimization to yield an energy minimized model; (c) remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the homolog of human constitutive androstane receptor (CAR).

The present invention also provides a method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising: (a) crystallizing the molecule or molecular complex; (b) generating an X-ray diffraction pattern from the crystallized molecule or molecular complex; (c) applying at least a portion of the structure coordinates set forth in Table 2 or Table 3 to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

The present invention also provides a method for attempting to make a crystallized complex comprising a polypeptide and a modulator having a molecular weight of less than 5 kDa, the method comprising: (a) crystallizing a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that

-16-

hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); such that crystals of the crystallized polypeptide will diffract X-rays to a resolution of 5 Å or better; and (b) soaking the crystals in a solution comprising a potential modulator having a molecular weight of less than 5 kDa.

The present invention also provides a method for incorporating a potential modulator in a crystal of a polypeptide, comprising placing a hexagonal crystal of human constitutive androstane receptor (CAR) having unit cell dimensions $a = 83.0 \text{ Å}$; $b = 116.8 \text{ Å}$; $c = 131.9 \text{ Å}$, $a = b = c = 90^\circ$, with an orthorhombic space group P212121, in a solution comprising the potential modulator.

The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprises structural coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about six amino acid residues from a druggable region of human constitutive androstane receptor (CAR).

The present invention also provides a scalable three-dimensional configuration of points, at least a portion of the points derived from some or all of the structure coordinates as listed in Table 2 or Table 3 for a plurality of amino acid residues from a druggable region of human constitutive androstane receptor (CAR). In one embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about five amino acid residues from a druggable region of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points. In another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone and optionally the side chain atoms of at least about ten amino acid residues from a druggable region of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points. In another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about fifteen amino acid residues from a druggable region of human constitutive androstane receptor

-17-

(CAR) are used to derive part or all of the portion of points. In another embodiment, substantially all of the points are derived from structure coordinates as listed in Table 2 or Table 3. In still another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points.

The present invention also provides a scalable three-dimensional configuration of points, comprising points having a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least five amino acid residues, wherein the five amino acid residues are from a druggable region of human constitutive androstane receptor (CAR). In one embodiment, any point-to-point distance, calculated from the three dimensional coordinates as listed in Table 2 or Table 3, between one of the backbone atoms for one of the five amino acid residues and another backbone atom of a different one of the five amino acid residues is not more than about 10 Å.

The present invention also provides a scalable three-dimensional configuration of points comprising points having a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR).

The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprise the identity and three-dimensional coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR).

The present invention also provides a scalable three-dimensional configuration of points, wherein the points have a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in

-18-

Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR), wherein up to one amino acid residue in each of the regions can have a conservative substitution thereof.

5 The present invention also provides a scalable three-dimensional configuration of points derived from a druggable region of a polypeptide, wherein the points have a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least ten amino acid residues that participate in the
10 intersubunit contacts of human constitutive androstane receptor (CAR).

 The present invention also provides a computer-assisted method for identifying an inhibitor of the activity of human constitutive androstane receptor (CAR), comprising: (a) supplying a computer modeling application with a set of structure coordinates as listed in Table 2 or Table 3 for the atoms
15 of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) supplying the computer modeling application with a set of structure coordinates of a chemical entity; and (c) determining whether the chemical entity is expected to bind to or interfere with the
20 molecule or complex. In one embodiment, determining whether the chemical entity is expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and a druggable region of the molecule or complex, followed by computationally analyzing the results of the fitting operation to quantify the association
25 between the chemical entity and the druggable region. In one embodiment, the method further comprises screening a library of chemical entities.

 The present invention also provides a computer-assisted method for designing an inhibitor of constitutive androstane receptor (CAR) activity comprising: (a) supplying a computer modeling application with a set of
30 structure coordinates having a root mean square deviation of less than about 1.5 Å from the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable

-19-

regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) supplying the computer modeling application with a set of structure coordinates for a chemical entity; (c) evaluating the potential binding interactions between the chemical entity and the molecule or complex; (d) structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and (e) determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity. In one embodiment, determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and the molecule or complex, followed by computationally analyzing the results of the fitting operation to evaluate the association between the chemical entity and the molecule or complex. In another embodiment, the set of structure coordinates for the chemical entity is obtained from a chemical library.

The present invention also provides a computer-assisted method for designing an inhibitor of constitutive androstane receptor (CAR) activity de novo comprising: (a) supplying a computer modeling application with a set of three-dimensional coordinates derived from the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) computationally building a chemical entity represented by a set of structure coordinates; and (c) determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex, wherein binding to or interfering with the molecule or complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity. In one embodiment, determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and a druggable region of the

-20-

molecule or complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the druggable region.

The present invention also provides a method for identifying a potential modulator for the prevention or treatment of a disease or disorder, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide comprising: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) obtaining a potential modulator for the prevention or treatment of a disease or disorder based on the three dimensional structure of the crystallized polypeptide; (c) contacting the potential modulator with a second polypeptide comprising: (i) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (ii) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (iii) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); which second polypeptide can optionally be the same as the crystallized polypeptide; and (d) assaying the activity of the second polypeptide, wherein a change in the activity of the second polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

The present invention also provides a method for designing a candidate modulator for screening for inhibitors of a polypeptide, the method comprising: (a) providing the three dimensional structure of a druggable region of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least

-21-

about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one
5 biological activity of human constitutive androstane receptor (CAR); and (b) designing a candidate modulator based on the three dimensional structure of the druggable region of the polypeptide.

The present invention also provides a method for identifying a potential modulator of a polypeptide from a database, the method comprising: (a)
10 providing the three-dimensional coordinates for a plurality of the amino acids of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that
15 hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) identifying a druggable region of the polypeptide; and (c) selecting from a database at least one potential modulator comprising three dimensional
20 coordinates which indicate that the modulator can bind or interfere with the druggable region. In one embodiment, the modulator is a small molecule.

The present invention also provides a method for preparing a potential modulator of a druggable region contained in a polypeptide, the method comprising: (a) using the atomic coordinates for the backbone atoms of at
25 least about six amino acid residues from a polypeptide of SEQ ID NO: 4, with a root mean square deviation from the backbone atoms of the amino acid residues of not more than 1.5 Å, to generate one or more three-dimensional structures of a molecule comprising a druggable region from the polypeptide; (b) employing one or more of the three dimensional structures of the molecule
30 to design or select a potential modulator of the druggable region; and (c) synthesizing or obtaining the modulator.

-22-

The present invention also provides an apparatus for determining whether a compound is a potential modulator of a polypeptide, the apparatus comprising: (a) a memory that comprises: (i) the three dimensional coordinates and identities of at least about fifteen atoms from a druggable region of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (ii) executable instructions; and (b) a processor that is capable of executing instructions to: (i) receive three-dimensional structural information for a candidate modulator; (ii) determine if the three-dimensional structure of the candidate modulator is complementary to the three dimensional coordinates of the atoms from the druggable region; and (iii) output the results of the determination.

The present invention also provides a method for making an inhibitor of constitutive androstane receptor (CAR) activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of constitutive androstane receptor (CAR) activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex comprising at least a portion of at least one druggable region from human constitutive androstane receptor (CAR); supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind or to interfere with the molecule or complex at a druggable region, wherein binding to or interfering with the molecule or complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity.

-23-

The present invention also provides a computer readable storage medium comprising digitally encoded data, wherein the data comprises structural coordinates for a druggable region that is structurally homologous to the structure coordinates as listed in Table 2 or Table 3 for a druggable region of human constitutive androstane receptor (CAR).

The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprise a majority of the three-dimensional structure coordinates as listed in Table 2 or Table 3. In one embodiment, the computer readable storage medium further comprises the identity of the atoms for the majority of the three-dimensional structure coordinates as listed in Table 2 or Table 3. In another embodiment, the data comprise substantially all of the three-dimensional structure coordinates as listed in Table 2 or Table 3.

The present invention also provides a method for building a model for an activated conformation of a constitutive androstane receptor (CAR), the method comprising: (a) employing coordinates for CAR residues 107 to 332 as shown in Table 2; (b) rotating and translating an X-ray structure of the Vitamin D receptor (VDR), so as to superimpose its core backbone atoms onto corresponding atoms from CAR; (c) combining a superimposed VDR AF2 helix, residues 416-423, with residues 107-332 from CAR from step (a), to provide a starting model for residues 107-332 and 341-348 of CAR in the activated conformation; (d) computationally mutating Val418, Leu419, Val421, Phe422 and Gly423 in the VDR AF2 helix to corresponding amino acids in a CAR AF2 helix, wherein the corresponding amino acids in the CAR AF2 helix are Leu343, Gln344, Ile346, Cys347 and Ser348, respectively; and (e) adjusting the conformations of the mutated amino acid side chains in residues 343, 344, and 346-348 of the AF2 helix of CAR to avoid overlaps, wherein the adjusting is accomplished by one of manual manipulation and conformational search and energy minimization. In one embodiment, the method further comprises modeling a CAR AF2 linker region, residues 333-340, by using a computational loop modeling technique.

-24-

Accordingly, it is an object of the present invention to provide a three-dimensional structure of the ligand-binding domain of CAR in complex with a ligand. The object is achieved in whole or in part by the present invention.

An object of the invention having been stated hereinabove, other
5 objects will be evident as the description proceeds, when taken in connection with the accompanying Drawings and Examples as described hereinbelow.

Brief Description of the Drawings

Figure 1 is a ribbon diagram depicting the secondary structure of CAR
10 LBD bound with ligand. The ligand is shown as ball and stick. Helices are indicated by H followed by the α helix number, and β -strands are indicated by **b** followed by the β -strand number. The line at the bottom of the figure indicates the scale, and corresponds to 50 angstroms. N refers to the N-terminus and C refers to the C-terminus.

15 Figure 2 is a structure-based sequence alignment of the human, mouse, and rat CAR polypeptides with the human PXR polypeptide and the human VDR polypeptide. The residues that make up the α helices are boxed with a light gray line and light gray background. The residues that make up the β sheets are boxed with a darker gray line and darker gray background.
20 The residues within 5Å of the ligand are individually boxed with a thin black square box. Conserved residues are indicated in bold type.

Figure 3 depicts the CAR ligand-binding site. CAR amino acids are shown with light and dark gray lines. A ligand is shown in heavy black lines. The hydrogen bonds between CAR amino acids and the ligand are shown
25 with dotted lines. Particular amino acids that are involved in the ligand binding are indicated using one letter code and amino acid number.

Figure 4 is a stick diagram depicting another view of the ligand-binding site. CAR amino acids are shown with light and dark gray lines. A ligand is shown in heavy black lines. The hydrogen bonds between CAR amino acids
30 and the ligand are shown with dotted lines. Particular amino acids that are involved in the ligand binding are indicated using one letter code and amino acid number.

-25-

Figure 5 depicts the CAR binding pocket. Ligand Compound 1 is shown in Van der Waals ball form. The binding pocket is shown as a dotted surface. The protein backbone is shown in ribbon form. The side chains in the binding pocket are shown in ball and stick form.

5 Figure 6 depicts another view of the ribbon diagram depicting secondary structure of the three-layer sandwich shaped ligand-binding pocket.

Figure 7 is a schematic diagram of a general strategy for synthesizing ligands that can bind to the CAR LBD. This scheme is described in Example
10 6, which outlines the synthesis of an exemplary ligand, Compound 1.

Brief Description of the Sequences in the Sequence Listing

SEQ ID NO: 1 is a DNA sequence encoding a full-length human CAR polypeptide.

15 SEQ ID NO: 2 is an amino acid sequence of a full-length human CAR polypeptide.

SEQ ID NO: 3 is a DNA sequence encoding human CAR residues 103-340, the ligand-binding domain of CAR polypeptide.

20 SEQ ID NO: 4 is an amino acid sequence of residues 103-340, the ligand-binding domain of CAR polypeptide.

SEQ ID NO: 5 is a His tag amino acid sequence.

25 SEQ ID NO: 6 is a DNA sequence of a primer used in combination with the primer of SEQ ID NO: 7 to amplify a DNA fragment encoding amino acid residues 103 - 348 of a human CAR polypeptide. In addition to amplifying these coding nucleotides, the primer also includes sequences that will result in the amplified product (a) encoding a His tag as in SEQ ID NO: 5; and (b) having an NdeI endonuclease restriction site (CATATG) just 5' to the His tag-encoding residues.

30 SEQ ID NO: 7 is a DNA sequence of a primer used in combination with the primer of SEQ ID NO: 6 to amplify a DNA fragment encoding residues 103 - 348 of a human CAR polypeptide. The sequence of this primer includes a BamHI endonuclease restriction site (GGATCC) 3' to the human CAR

-26-

polypeptide coding residues. When this primer is used in combination with the primer of SEQ ID NO: 6, the amplified product will have the following arrangement of features: NdeI site – His tag – nucleotides encoding human CAR amino acids 103 to 348 – BamHI site.

5

Detailed Description of the Invention

Until disclosure of the present invention presented herein, the ability to obtain crystalline forms of a CAR LBD, particularly in complex with an antagonist ligand, has not been realized. And until disclosure of the present invention presented herein, a detailed three-dimensional crystal structure of an unliganded CAR polypeptide or a CAR polypeptide in complex with a ligand has not been solved.

In addition to providing structural information, crystalline polypeptides provide other advantages. For example, the crystallization process itself further purifies the polypeptide, and satisfies one of the classical criteria for homogeneity. In fact, crystallization frequently provides unparalleled purification quality, removing impurities that are not removed by other purification methods such as HPLC, dialysis, conventional column chromatography, etc. Moreover, crystalline polypeptides are often stable at ambient temperatures and free of protease contamination and degradation associated with solution storage. Crystalline polypeptides can also be useful as pharmaceutical preparations. Finally, crystallization techniques are generally free of problems such as denaturation associated with other stabilization methods (e.g., lyophilization).

Once crystallization has been accomplished, crystallographic data provides useful structural information that can assist the design of compounds that can serve as agonists or antagonists, as described herein below. In addition, the crystal structure provides information that can be used to map the molecular surface of the ligand-binding domain of CAR. A small non-peptide molecule designed to mimic portions of this surface could serve as a modulator of CAR activity.

-27-

I. Definitions

Before the present proteins, nucleotide sequences, and methods are described, it is understood that this invention is not limited to the particular methodology, protocols, cell lines, vectors, and reagents described, as these
5 can vary. It is also to be understood that the terminology used herein is for the purpose of describing particular embodiments only, and is not intended to limit the scope of the present invention, the invention being defined by the claims.

Unless defined otherwise, all technical and scientific terms used herein
10 are intended to have their ordinary meanings as understood by one of ordinary skill in the art to which this invention pertains. Although any methods and materials similar or equivalent to those described herein can be used in the practice or testing of the present invention, representative methods, devices, and materials are now described. All publications mentioned herein
15 are incorporated by reference for the purpose of describing the cell lines, vectors, reagents, and methodologies they disclose.

Following long-standing patent law convention, the articles "a" and "an" are used herein to refer to one or to more than one (*i.e.*, to at least one) of the grammatical object of the article. By way of example, "an element" means
20 one element or more than one element.

As used herein, the term "AF2 helix" refers to a short alpha-helix, usually including 5-8 residues, located at the C-terminal end of a LBD sequence, that can usually adopt multiple positions, orientations, and conformations in the structure, and which is involved in binding to
25 coactivators. In the hypothetical activated conformation of CAR, the AF2 helix is expected to include residues 341 to 347. These residues do not adopt an alpha-helical conformation in the structure of CAR bound to Compound 1.

As used herein, the terms "Compound 1" and "Formula (A)" are used interchangeably and refer to 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-
30 benzimidazole-6-carboxamide.

As used herein, the term "AF2 glutamate" refers to a glutamate residue in the AF2 helix that can make hydrogen bond interactions with the exposed

-28-

NH groups of the LXXLL-containing peptide from a coactivator if the AF2 helix is in the active position. In CAR, the AF2 glutamate is residue number 345.

As used herein, the terms "activated", "active conformation", and "activated conformation" of an LBD are used interchangeably and refer to a conformation where the AF2 helix is in the active position, thereby placing the AF2 glutamate residue in a position and orientation that creates a charge clamp that can recruit coactivator peptides. Similarly, the terms "active position of the AF2 helix" and "active conformation of the AF2 helix" are used interchangeably and mean an AF2 helix having a position and/or orientation similar to that of the AF2 helix in the PPAR γ /SRC-1/rosiglitazone structure of Nolte *et al.*, 1998, allowing the AF2 glutamate residue to make interactions with the exposed NH groups of a coactivator peptide. The position and/or orientation of the AF2 helix in an NR structure can be compared with that of the AF2 helix in another NR structure by rotating and/or translating one structure so as to superimpose the backbone atoms of helices 1 through 10 onto the corresponding atoms of the other structure, where corresponding residues are determined by sequence alignment. If, after superimposition, a majority of the backbone atoms of the core of the AF2 helix lie within 2.0 angstroms of the corresponding atoms from the PPAR γ /SRC-1/rosiglitazone structure, then the AF2 helix is defined as being in an active position or active conformation.

Other examples of a nuclear receptor where the AF2 helix is in an "active position" include the X-ray structures of the estrogen receptor α (ER α) bound to estradiol (Brzozowski *et al.*, 1997) and diethylstilbesterol (DES) (Shiau *et al.*, 1998). Examples of a nuclear receptor where the AF2 helix is not in an "active position" are the X-ray structures of the estrogen receptor α (ER α) bound to raloxifene (Brzozowski *et al.*, 1997) and tamoxifen (Shiau *et al.*, 1998). Binding of a coactivator, and AF2-dependent activation of gene transcription, normally requires that the AF2 helix be in the "active position" (Nolte *et al.*, 1998; Shiau *et al.*, 1998). This creates a "charge-clamp" structure that holds the coactivator in its required position (Nolte *et al.*, 1998).

-29-

As used herein, the terms "repressed", "inactive conformation", and "repressed conformation" of an LBD are used interchangeably and refer to a conformation where the AF2 helix is not in the active position, and where the AF2 glutamate residue is not in a position that could create the charge clamp that can recruit coactivator peptides.

As used herein, the term "agonist" refers to an agent that supplements or potentiates the biological activity of a functional CAR gene or protein, or of a polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide and/or a polypeptide encoded by a gene that contains a CAR binding site or response element in its promoter region. An agent is also an agonist when the changes in gene expression, considered over many genes, are similar in direction to those induced by other agents that are commonly regarded as agonists. In one embodiment, an agonist of CAR is an androstane.

As used herein, the term "antagonist" refers to an agent that decreases or inhibits the biological activity of a functional gene or protein (for example, a functional CAR gene or protein), or that supplements or potentiates the biological activity of a naturally occurring or engineered non-functional gene or protein (for example, a non-functional CAR gene or protein). Alternatively, an antagonist can decrease or inhibit the biological activity of a functional gene or polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide and/or contains a CAR binding site or response element in its promoter region. An antagonist can also supplement or potentiate the biological activity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide, and/or contains a CAR binding site or response element in its promoter region. An agent is also an antagonist when the changes in gene expression, considered over many genes, are opposite in direction to those induced by other agents that are commonly regarded as agonists.

As used herein, the terms " α -helix" and "alpha-helix" are used interchangeably and refer to a conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a

-30-

left-handed or right-handed direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turn of the helix, which extends about 0.56 nm along the long axis.

5 As used herein, the terms "amino acid", "amino acid residue", and "residue" are used interchangeably and refer to an amino acid formed upon chemical digestion (hydrolysis) of a peptide or polypeptide at its peptide linkages. Amino acids can also be synthesized individually or as components of a peptide. In one embodiment, the amino acid residues described herein
10 are in the "L" isomeric form. However, residues in the "D" isomeric form can be substituted for any L-amino acid residue, provided that the desired functional property is retained by the polypeptide. In the context of an amino acid, NH_2 refers to the free amino group present at the amino terminus of a polypeptide, although some amino acids can have NH_2 groups at other
15 positions in the amino acid. COOH refers to the free carboxy group present at the carboxy terminus of a polypeptide. In keeping with standard polypeptide nomenclature, abbreviations for amino acid residues are presented above. The term "amino acid" is intended to embrace all molecules, whether natural or synthetic, which include both an amino functionality and an acid
20 functionality and capable of being included in a polymer of naturally occurring amino acids. Exemplary amino acids include naturally occurring amino acids; analogs, derivatives and congeners thereof; amino acid analogs having variant side chains; and all stereoisomers of any of the foregoing.

 It is noted that amino acid residue sequences represented herein by
25 formulae have a left-to-right orientation in the conventional direction of amino terminus to carboxy terminus. In addition, the terms "amino acid", "amino acid residue", and "residue" are broadly defined to include the amino acids listed in the above table and modified or unusual amino acids. Furthermore, it is noted that a dash at the beginning or end of an amino acid residue sequence
30 indicates a peptide bond to a further sequence of one or more amino acid residues or a covalent bond to an amino-terminal group such as NH_2 or acetyl or to a carboxy-terminal group such as COOH .

-31-

As used herein, the terms "β-sheet" and "beta-sheet" are used interchangeably and refer to the conformation of a polypeptide chain stretched into an extended zigzag conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "anti-parallel" run in the opposite direction from the parallel chains or from each other.

The term "binding" refers to an association, which can be a stable association, between two molecules, *i.e.*, between a polypeptide of the invention and a binding partner, due to, for example, electrostatic, hydrophobic, ionic, and/or hydrogen-bond interactions under physiological conditions.

As used herein, the terms "binding pocket of the CAR ligand-binding domain", "CAR ligand-binding pocket" and "CAR binding pocket" are used interchangeably, and refer to the large cavity within the CAR ligand-binding domain where a ligand (*e.g.* Compound 1) binds. This cavity can be empty, or can contain water molecules or other molecules from the solvent, or can contain ligand atoms. The "main" binding pocket includes the region of space not occupied by atoms of CAR that is approximately encompassed or bounded by residues Phe132, Phe161, Ile164, Asn165, Thr166, Met168, Val169, Ala198, Val199, Cys202, His203, Leu206, Phe217, Tyr224, Thr225, Ile226, Glu227, Asp228, Gly229, Ala230, Phe234, Phe238, Leu239, Leu242, Phe243, His246, Tyr326, Ile330, Leu336, Ser337, Met339, and Met340. The binding pocket also includes small regions near to and contiguous with the "main" binding pocket that not occupied by atoms of CAR.

As used herein the term "biological activity" refers to any biochemical function of a biological molecule. A biological activity includes, but is not limited to, an interaction with another biological molecule (for example, a polypeptide or a nucleic acid, or a combination thereof). As such, a biological activity results in a biochemical effect including, but not limited to the initiation or inhibition of transcription of a gene.

The term "complex" refers to an association between at least two moieties (*i.e.* chemical or biochemical) that have an affinity for one another.

-32-

Examples of complexes include associations between antigen/antibodies, lectin/avidin, target polynucleotide/probe oligonucleotide, antibody/anti-antibody, receptor/ligand, enzyme/ligand, polypeptide/ polypeptide, polypeptide/polynucleotide, polypeptide/co-factor, polypeptide/substrate, 5 polypeptide/inhibitor, polypeptide/small molecule, and the like. "Member of a complex" refers to one moiety of the complex, such as an antigen or ligand. "Protein complex" or "polypeptide complex" refers to a complex comprising at least one polypeptide.

The term "conserved residue" refers to an amino acid that is a member 10 of a group of amino acids having certain common properties. The term "conservative amino acid substitution" refers to the substitution (conceptually or otherwise) of an amino acid from one such group with a different amino acid from the same group. A functional way to define common properties between individual amino acids is to analyze the normalized frequencies of 15 amino acid changes between corresponding proteins of homologous organisms (Schulz & Schirmer, 1979). According to such analyses, groups of amino acids can be defined where amino acids within a group exchange preferentially with each other, and therefore resemble each other most in their impact on the overall protein structure (Schulz & Schirmer, 1979). 20 Representative examples of sets of amino acid groups defined in this manner include: (i) a charged group, consisting of Glu and Asp, Lys, Arg and His, (ii) a positively-charged group, consisting of Lys, Arg and His, (iii) a negatively-charged group, consisting of Glu and Asp, (iv) an aromatic group, consisting of Phe, Tyr and Trp, (v) a nitrogen ring group, consisting of His and Trp, (vi) a 25 large aliphatic nonpolar group, consisting of Val, Leu and Ile, (vii) a slightly-polar group, consisting of Met and Cys, (viii) a small-residue group, consisting of Ser, Thr, Asp, Asn, Gly, Ala, Glu, Gln and Pro, (ix) an aliphatic group consisting of Val, Leu, Ile, Met and Cys, and (x) a small hydroxyl group consisting of Ser and Thr.

30 As used herein, the term "DNA segment" refers to a DNA molecule that has been isolated free of total genomic DNA of a particular species. In one embodiment, a DNA segment encoding a CAR polypeptide refers to a nucleic

-33-

acid comprising SEQ ID NO: 1. In another embodiment, a DNA segment encoding a CAR polypeptide refers to a nucleic acid comprising SEQ ID NO: 3. DNA segments can comprise a portion of a recombinant vector, including, for example, a plasmid, a cosmid, a phage, a virus, and the like.

5 As used herein, the term "DNA sequence encoding a CAR polypeptide" refers to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in amino acid sequence of
10 the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes can be identical or can have certain modifications, including nucleotide substitutions, additions, or deletions, all of which still code for polypeptides
15 having substantially the same activity.

The term "domain", when used in connection with a polypeptide, refers to a specific region within the polypeptide that comprises a particular structure or mediates a particular function. In the typical case, a domain of a polypeptide of the invention is a fragment of the polypeptide. In certain
20 instances, a domain is a structurally stable domain, as evidenced, for example, by mass spectroscopy, or by the fact that a modulator can bind to a druggable region of the domain. In one embodiment, a domain of a CAR polypeptide is a ligand-binding domain. In another embodiment, a domain of a CAR polypeptide is a DNA-binding domain.

25 The term "druggable region", when used in reference to a polypeptide, nucleic acid, complex and the like, refers to a region of the molecule that is a target or is a likely target for binding a modulator. For a polypeptide, a druggable region generally refers to a region wherein several amino acids of a polypeptide would be capable of interacting with a modulator or other
30 molecule. For a polypeptide or complex thereof, exemplary druggable regions including binding pockets and sites, enzymatic active sites, interfaces between domains of a polypeptide or complex, surface grooves or contours or

-34-

surfaces of a polypeptide or complex which are capable of participating in interactions with another molecule. In certain instances, the interacting molecule is another polypeptide, which can be naturally occurring. In other instances, the druggable region is on the surface of the molecule. In one
5 embodiment, a druggable region of a CAR polypeptide comprises the binding site defined by amino acid residues 103-340. In another embodiment, a druggable region of a CAR polypeptide comprises amino acid residues and surfaces of the CAR polypeptide that interact with a RXR polypeptide during CAR-RXR heterodimer formation. In another embodiment, a druggable
10 region of a CAR polypeptide comprises the AF2 helix. In another embodiment, a druggable region of a CAR polypeptide comprises Glu345. In still another embodiment, a druggable region of a CAR polypeptide comprises a DNA-binding domain.

Druggable regions can be described and characterized in a number of
15 ways. For example, a druggable region can be characterized by some or all of the amino acids that make up the region, or the backbone atoms thereof, or the side chain atoms thereof (optionally with or without the C α atoms). Alternatively, in certain instances, the volume of a druggable region corresponds to that of a carbon based molecule of at least about 200 atomic
20 mass units (amu) and often up to about 800 amu. In other instances, it will be appreciated that the volume of such region can correspond to a molecule of at least about 600 amu and often up to about 1600 amu or more.

Alternatively, a druggable region can be characterized by comparison to other regions on the same or other molecules. For example, the term
25 "affinity region" refers to a druggable region on a molecule (such as a polypeptide of the invention) that is present in several other molecules, in so much as the structures of the same affinity regions are sufficiently the same so that they are expected to bind the same or related structural analogs. An example of an affinity region is an ATP-binding site of a protein kinase that is
30 found in several protein kinases (whether or not of the same origin). Another example of an affinity region is a DNA-binding domain: for example, the DNA-binding domain of a CAR polypeptide.

-35-

In contrast to an affinity region, the term "selectivity region" refers to a druggable region of a molecule that can not be found on other molecules, in so much as the structures of different selectivity regions are sufficiently different so that they are not expected to bind the same or related structural analogs. An exemplary selectivity region is a catalytic domain of a protein kinase that exhibits specificity for one substrate. In certain instances, a single modulator can bind to the same affinity region across a number of proteins that have a substantially similar biological function, whereas the same modulator can bind to only one selectivity region of one of those proteins.

Continuing with examples of different druggable regions, the term "undesired region" refers to a druggable region of a molecule that upon interacting with another molecule results in an undesirable affect. For example, a binding site that oxidizes the interacting molecule and thereby results in increased toxicity for the oxidized molecule can be deemed an "undesired region". Other examples of potential undesired regions include regions that upon interaction with a drug decrease the membrane permeability of the drug, increase the excretion of the drug, or increase the blood brain transport of the drug. It can be the case that, in certain circumstances, an undesired region will no longer be deemed an undesired region because the affect of the region will be favorable, *i.e.*, a drug intended to treat a brain condition would benefit from interacting with a region that resulted in increased blood brain transport, whereas the same region could be deemed undesirable for drugs that were not intended to be delivered to the brain.

When used in reference to a druggable region, the "selectivity" or "specificity" of a molecule such as a modulator to a druggable region can be used to describe the binding between the molecule and a druggable region. For example, the selectivity of a modulator with respect to a druggable region can be expressed by comparison to another modulator, using the respective values of K_d (*i.e.*, the dissociation constants for each modulator-druggable region complex) or, in cases where a biological effect is observed below the K_d , the ratio of the respective EC_{50} 's (*i.e.*, the concentrations that produce

-36-

50% of the maximum response for the modulator interacting with each druggable region).

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced. As such, the term "expression" generally includes those cellular processes that begin with transcription and end with the production of a functional polypeptide. As used herein, "expression" is also intended to refer to cellular processes by which a polypeptide is produced that would otherwise be functional except for the presence of mutations in the nucleotide sequence encoding it. Consistent with this usage, "expression" includes, but is not limited to, such processes as transcription, translation, post-translational modification, and transport of a polypeptide.

A "fusion protein" or "fusion polypeptide" refers to a chimeric protein as that term is known in the art and can be constructed using methods known in the art. In many examples of fusion proteins, there are two different polypeptide sequences, and in certain cases, there can be more. The sequences can be linked in frame. A fusion protein can include a domain that is found (albeit in a different protein) in an organism that also expresses the first protein, or it can be an "interspecies", "intergenic", etc. fusion expressed by different kinds of organisms. In various embodiments, the fusion polypeptide can comprise one or more amino acid sequences linked to a first polypeptide. In the case where more than one amino acid sequence is fused to a first polypeptide, the fusion sequences can be multiple copies of the same sequence, or alternatively, can be different amino acid sequences. The fusion polypeptides can be fused to the N-terminus, the C-terminus, or the N- and C-terminus of the first polypeptide. Exemplary fusion proteins include polypeptides comprising a glutathione S-transferase tag (GST-tag), histidine tag (His-tag), an immunoglobulin domain, or an immunoglobulin-binding domain.

As used herein, the term "gene" is used for simplicity to refer to a nucleotide sequence that encodes a protein, a polypeptide, or a peptide. As such, the term "gene" refers to a nucleic acid comprising an open reading

-37-

frame encoding a polypeptide having exon sequences and, optionally, intron sequences. The term "intron" refers to a DNA sequence present in a given gene that is not translated into protein and is generally found between exons. As will be understood by those of skill in the art, this functional term includes
5 both genomic sequences and cDNA sequences. Representative embodiments of such sequences are disclosed herein.

The term "having substantially similar biological activity", when used in reference to two polypeptides, refers to a biological activity of a first polypeptide which is substantially similar to at least one of the biological
10 activities of a second polypeptide. A substantially similar biological activity means that the polypeptides carry out a similar function, *i.e.*, a similar enzymatic reaction or a similar physiological process, etc. For example, two homologous proteins can have a substantially similar biological activity if they are involved in a similar enzymatic reaction, *i.e.*, they are both kinases which
15 catalyze phosphorylation of a substrate polypeptide, however, they can phosphorylate different regions on the same protein substrate or different substrate proteins altogether. Alternatively, two homologous proteins can also have a substantially similar biological activity if they are both involved in a similar physiological process, *i.e.*, regulation of transcription. For example,
20 two proteins can be transcription factors, however, they can bind to different DNA sequences or bind to different polypeptide interactors. Substantially similar biological activities can also be associated with proteins carrying out a similar structural role, for example, two membrane proteins.

As used herein, the term "interact" refers to detectable interactions
25 between molecules, such as can be detected using, for example, a yeast two-hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions include, but are not limited to protein-protein, protein-nucleic acid, and protein-small molecule interactions. These interactions can be in the form of covalent or non-covalent interactions
30 including, but not limited to ionic, hydrogen bonding, and van der Waals interactions.

-38-

As used herein, the term "isolated" refers to a nucleic acid substantially free of other nucleic acids, proteins, lipids, carbohydrates, or other materials with which it can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide is substantially free of nucleic acids, carbohydrates, lipids, and other undesired polypeptides. The term "isolated polypeptide" refers to a polypeptide, in certain embodiments prepared from recombinant DNA or RNA, or of synthetic origin, or some combination thereof, which (1) is not associated with proteins that it is normally found with in nature, (2) is isolated from the cell in which it normally occurs, (3) is isolated free of other proteins from the same cellular source, (4) is expressed by a cell from a different species, or (5) does not occur in nature.

The term "isolated nucleic acid" refers to a polynucleotide of genomic, cDNA, or synthetic origin or some combination thereof, which (1) is not associated with the cell in which the "isolated nucleic acid" is found in nature, or (2) is operably linked to a polynucleotide to which it is not linked in nature.

The terms "label" or "labeled" refer to incorporation or attachment, optionally covalently or non-covalently, of a detectable marker into a molecule, such as a polypeptide. Various methods of labeling polypeptides are known in the art and can be used. Examples of labels for polypeptides include, but are not limited to the following: radioisotopes, fluorescent labels, heavy atoms, enzymatic labels or reporter genes, chemiluminescent groups, biotinyl groups, predetermined polypeptide epitopes recognized by a secondary reporter (*i.e.*, leucine zipper pair sequences, binding sites for secondary antibodies, metal binding domains, epitope tags). Examples and use of such labels are well known by the skilled artisan. In some embodiments, spacer arms of various lengths can be attached to labels to reduce potential steric hindrance.

The term "mammal" is known in the art, and exemplary mammals include humans, primates, bovines, porcines, canines, felines, and rodents (*i.e.*, mice and rats).

-39-

The term "modulation", when used in reference to a functional property or biological activity or process (*i.e.*, enzyme activity or receptor binding), refers to the capacity to up regulate (*i.e.*, activate or stimulate), down regulate (*i.e.*, inhibit or suppress), or otherwise change a quality of such property, activity, or process. In certain instances, such regulation can be contingent on the occurrence of a specific event, such as activation of a signal transduction pathway, and/or can be manifest only in particular cell types.

The term "modulator" refers to a polypeptide, nucleic acid, macromolecule, complex, molecule, small molecule, compound, species, or the like (naturally-occurring or non-naturally-occurring), or an extract made from biological materials such as bacteria, plants, fungi, or animal cells or tissues, that can be capable of causing modulation. Modulators can be evaluated for potential activity as inhibitors or activators (directly or indirectly) of a functional property, biological activity or process, or combination thereof, (*i.e.*, agonist, partial antagonist, partial agonist, inverse agonist, antagonist, anti-microbial agents, inhibitors of microbial infection or proliferation, and the like) by inclusion in assays. In such assays, many modulators can be screened at one time. The activity of a modulator can be known, unknown, or partially known.

As used herein, the term "molecular replacement" refers to a method that involves generating a preliminary model of the wild-type CAR ligand-binding domain, or a CAR mutant crystal the structure for which coordinates are unknown, by orienting and positioning a molecule the structure for which coordinates are known (*e.g.*, the vitamin D receptor; VDR) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure the coordinates for which are unknown. This, in turn, can be subjected to any of the several forms of refinement known in the art to provide a final, accurate structure of the unknown crystal (see *e.g.* Lattman, 1985; Rossmann, 1972). Using the structure coordinates of the ligand-binding domain of CAR provided by this invention, molecular

-40-

replacement can be used to determine the structure coordinates of a crystal of a mutant or of a homologue of the CAR ligand-binding domain, or of a different crystal form of the CAR ligand-binding domain.

5 The term "motif" refers to an amino acid sequence that is commonly found in a protein of a particular structure or function. Typically, a consensus sequence is defined to represent a particular motif. The consensus sequence need not be strictly defined and can contain positions of variability, degeneracy, variability of length, etc. The consensus sequence can be used to search a database to identify other proteins that can have a similar
10 structure or function due to the presence of the motif in its amino acid sequence. For example, on-line databases can be searched with a consensus sequence in order to identify other proteins containing a particular motif. Various search algorithms and/or programs can be used, including FASTA, BLAST, or ENTREZ. FASTA and BLAST are available as a part of
15 the GCG sequence analysis package (Accelrys, Inc., San Diego, California, United States of America). ENTREZ is available through the National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, Maryland, United States of America.

20 As used herein, the term "mutation" carries its traditional connotation and refers to a change, inherited, naturally occurring, or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art.

The term "naturally occurring", as applied to an object, refers to the fact that an object can be found in nature. For example, a polypeptide or
25 polynucleotide sequence that is present in an organism (including bacteria) that can be isolated from a source in nature and which has not been intentionally modified by man in the laboratory is naturally occurring.

The term "nucleic acid" refers to a polymeric form of nucleotides, either ribonucleotides or deoxynucleotides or a modified form of either type of
30 nucleotide. The terms should also be understood to include, as equivalents, analogs of either RNA or DNA made from nucleotide analogs, and, as

-41-

applicable to the embodiment being described, single-stranded (such as sense or antisense) and double-stranded polynucleotides.

The term "nucleic acid of the invention" refers to a nucleic acid encoding a polypeptide of the invention, *i.e.*, a nucleic acid comprising a sequence consisting of, or consisting essentially of, the polynucleotide sequence set forth in SEQ ID NO: 1 or SEQ ID NO: 3. A nucleic acid of the invention can comprise all, or a portion of: the nucleotide sequence of SEQ ID NO: 1 or SEQ ID NO: 3; a nucleotide sequence at least 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98% or 99% identical to SEQ ID NO: 1 or SEQ ID NO: 3; a nucleotide sequence that hybridizes under stringent conditions to SEQ ID NO: 1 or SEQ ID NO: 3; nucleotide sequences encoding polypeptides that are functionally equivalent to polypeptides of the invention; nucleotide sequences encoding polypeptides at least about 60%, 70%, 80%, 85%, 90%, 95%, 98%, 99% homologous or identical with an amino acid sequence of SEQ ID NO: 2 or SEQ ID NO: 4; nucleotide sequences encoding polypeptides having an activity of a polypeptide of the invention and having at least about 60%, 70%, 80%, 85%, 90%, 95%, 98%, 99% or more homology or identity with SEQ ID NO: 2 or SEQ ID NO: 4; nucleotide sequences that differ by 1 to about 2, 3, 5, 7, 10, 15, 20, 30, 50, 75 or more nucleotide substitutions, additions or deletions, such as allelic variants, of SEQ ID NO: 1 and SEQ ID NO: 3; nucleic acids derived from and evolutionarily related to SEQ ID NO: 1 or SEQ ID NO: 3; and complements of and nucleotide sequences resulting from the degeneracy of the genetic code, for all of the foregoing and other nucleic acids of the invention. Nucleic acids of the invention also include homologs, *i.e.*, orthologs and paralogs, of SEQ ID NO: 1 or SEQ ID NO: 3 and also variants of SEQ ID NO: 1 or SEQ ID NO: 3 which have been codon optimized for expression in a particular organism (*i.e.*, host cell).

The term "operably linked", when describing the relationship between two nucleic acid regions, refers to a juxtaposition wherein the regions are in a relationship permitting them to function in their intended manner. For example, a control sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under

-42-

conditions compatible with the control sequences, such as when the appropriate molecules (*i.e.*, inducers and polymerases) are bound to the control or regulatory sequence(s).

As used herein, "orthorhombic unit cell" refers to a unit cell wherein a
5 $a \neq b \neq c$, and $\alpha = \beta = \gamma = 90^\circ$. The vectors a , b , and c describe the unit cell edges and the angles α , β , and γ describe the unit cell angles.

As used herein, the term "CAR" refers to any polypeptide with an amino acid sequence that can be aligned with at least one of human, mouse, or rat CAR, such that at least 50% of the amino acids are identical to the
10 corresponding amino acid in the human, mouse, or rat CAR. The term "CAR" also encompasses nucleic acids for which the corresponding translated protein sequence can be considered to be a CAR. The term "CAR" includes vertebrate homologs of CAR family members including, but not limited to mammalian and avian homologs. Representative mammalian homologs of
15 CAR family members include, but are not limited to murine and human homologs.

As used herein, the terms "CAR gene" and "recombinant CAR gene" are used interchangeably and refer to a nucleic acid molecule comprising an open reading frame encoding a CAR polypeptide, including both exon and
20 (optionally) intron sequences.

As used herein, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" are used interchangeably and refer to peptides having amino acid sequences which are substantially identical to native CAR amino acid sequences from the organism of interest and which
25 are biologically active in that they comprise all or a part of the amino acid sequence of a CAR polypeptide, or cross-react with antibodies raised against a CAR polypeptide, or retain all or some of the biological activity (*e.g.*, DNA or ligand-binding ability and/or dimerization ability) of the native amino acid sequence or protein. Such biological activity can include immunogenicity.

30 As used herein, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" are used interchangeably and refer to a subtype of the CAR family. In one embodiment, a CAR gene product is CAR.

-43-

In another embodiment, a CAR gene product comprises the amino acid sequence of SEQ ID NO: 2.

As used herein, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" also include analogs of a CAR polypeptide.

5 By "analog" is intended that a DNA or peptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences as are disclosed herein or those from other organisms, or can be created synthetically. Those skilled in the art will
10 appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct CAR analogs. There is no need for a "CAR gene product", "CAR protein", "CAR polypeptide", or "CAR peptide" to comprise all or substantially all of the amino acid sequence of a CAR polypeptide gene product. Shorter or longer sequences are anticipated to be
15 of use in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" also include fusion or recombinant CAR polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein and are known in the
20 art.

The term "phenotype" refers to the entire physical, biochemical, and physiological makeup of a cell, *i.e.*, having any one trait or any group of traits.

As used herein, the term "polypeptide" refers to any polymer comprising any of the 20 protein amino acids, regardless of its size. Although
25 "protein" is often used in reference to relatively large polypeptides and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides, and proteins, unless otherwise noted. As used herein, the terms "protein", "polypeptide" and "peptide" are used
30 interchangeably herein when referring to a gene product. The term "polypeptide", and the terms "protein" and "peptide" which are used interchangeably herein, refers to a polymer of amino acids. Exemplary

-44-

polypeptides include gene products, naturally occurring proteins, homologs, orthologs, paralog, fragments, as well as other equivalents, variants, and analogs of the foregoing.

5 The terms "polypeptide fragment" or "fragment", when used to refer to a reference polypeptide, refers to a polypeptide in which amino acid residues are deleted as compared to the reference polypeptide itself, but where the remaining amino acid sequence is usually identical to the corresponding positions in the reference polypeptide. Such deletions can occur at the amino-terminus or carboxy-terminus of the reference polypeptide, or
10 alternatively both. Fragments typically are at least 5, 6, 8 or 10 amino acids long, at least 14 amino acids long, at least 20, 30, 40 or 50 amino acids long, at least 75 amino acids long, or at least 100, 150, 200, 300, 500 or more amino acids long. A fragment can retain one or more of the biological activities of the reference polypeptide. In certain embodiments, a fragment
15 can comprise a druggable region, and optionally additional amino acids on one or both sides of the druggable region, which additional amino acids can number from 5, 10, 15, 20, 30, 40, 50, or up to 100 or more residues. Further, fragments can include a sub-fragment of a specific region, which sub-fragment retains a function of the region from which it is derived. In one
20 embodiment, a fragment can have immunogenic properties.

The term "polypeptide of the invention" refers to a polypeptide comprising the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4, or an equivalent or fragment thereof: *i.e.*, a polypeptide comprising a sequence consisting of, or consisting essentially of, the amino acid sequence
25 set forth in SEQ ID NO: 2 or SEQ ID NO: 4. Polypeptides of the invention include polypeptides comprising all or a portion of the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4 with 1 to about 2, 3, 5, 7, 10, 15, 20, 30, 50, 75 or more conservative amino acid substitutions; an amino acid
30 sequence that is at least 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98%, or 99% identical to SEQ ID NO: 2 or SEQ ID NO: 4; and functional fragments

-45-

thereof. Polypeptides of the invention also include homologs, *i.e.*, orthologs and paralogs, of SEQ ID NO: 2 or SEQ ID NO: 4.

As used herein, the term "primer" refers to a nucleic acid comprising in one embodiment 2 or more deoxyribonucleotides or ribonucleotides, in
5 another embodiment more than 3, in another embodiment more than 8, and in yet another embodiment at least about 20 nucleotides of an exonic or intronic region. In one embodiment, an oligonucleotide is between 10 and 30 bases in length.

The term "purified" refers to an object species that is the predominant
10 species present (*i.e.*, on a molar basis it is more abundant than any other individual species in the composition). A "purified fraction" is a composition wherein the object species comprises at least about 50 percent (on a molar basis) of all species present. In making the determination of the purity of a
15 species in solution or dispersion, the solvent or matrix in which the species is dissolved or dispersed is usually not included in such determination; instead, only the species (including the one of interest) dissolved or dispersed are taken into account. Generally, a purified composition will have one species that comprises more than about 80 percent of all species present in the composition, more than about 85%, 90%, 95%, 99% or more of all species
20 present. The object species can be purified to essential homogeneity (contaminant species cannot be detected in the composition by conventional detection methods) wherein the composition consists essentially of a single species. A skilled artisan can purify a polypeptide of the invention using standard techniques for protein purification in light of the teachings herein.
25 Purity of a polypeptide can be determined by a number of methods known to those of skill in the art, including for example, amino-terminal amino acid sequence analysis, gel electrophoresis, mass-spectrometry analysis and the methods described herein.

The terms "recombinant protein" and "recombinant polypeptide" refer to
30 a polypeptide that is produced by recombinant DNA techniques. An example of such techniques includes when DNA encoding a polypeptide is inserted

-46-

into a suitable expression vector that is in turn used to transform a host cell to produce the polypeptide encoded by the DNA.

A "reference sequence" is a defined sequence used as a basis for a sequence comparison. A reference sequence can be a subset of a larger sequence, for example, as a segment of a full-length protein given in a sequence listing such as SEQ ID NO: 2 or SEQ ID NO: 4, or can comprise a complete protein sequence. Generally, a reference sequence is at least 200, 300 or 400 nucleotides in length, frequently at least 600 nucleotides in length, and often at least 800 nucleotides in length (or the protein equivalent if it is shorter or longer in length). Because two proteins can each (1) comprise a sequence (*i.e.*, a portion of the complete protein sequence) that is similar between the two proteins, and (2) can further comprise a sequence that is divergent between the two proteins, sequence comparisons between two (or more) proteins are typically performed by comparing sequences of the two proteins over a "comparison window" to identify and compare local regions of sequence similarity.

A "comparison window," as used herein, refers to a conceptual segment of at least 20 contiguous amino acid positions wherein a protein sequence can be compared to a reference sequence of at least 20 contiguous amino acids and wherein the portion of the protein sequence in the comparison window can comprise additions or deletions (*i.e.*, gaps) of 20 percent or less as compared to the reference sequence (which does not comprise additions or deletions) for optimal alignment of the two sequences. Optimal alignment of sequences for aligning a comparison window can be conducted by the local homology algorithm of Smith & Waterman, 1981, by the homology alignment algorithm of Needleman & Wunsch, 1970, by the search for similarity method of Pearson & Lipman, 1988, by computerized implementations of these algorithms (GAP, BESTFIT, FASTA, and TFASTA in the Wisconsin Genetics Software Package, available from Accelrys, Inc., San Diego, California, United States of America), or by inspection, and the best alignment (*i.e.*, resulting in the highest percentage of homology over the comparison window) generated by the various methods can be identified.

-47-

The term "regulatory sequence" is a generic term used throughout the specification to refer to polynucleotide sequences, such as initiation signals, enhancers, regulators and promoters, that are necessary or desirable to affect the expression of coding and non-coding sequences to which they are operably linked. Exemplary regulatory sequences are described in Goeddel, 1990, and include, for example, the early and late promoters of SV40, adenovirus or cytomegalovirus immediate early promoter, the lac system, the trp system, the TAC or TRC system, T7 promoter whose expression is directed by T7 RNA polymerase, the major operator and promoter regions of phage lambda, the control regions for fd coat protein, the promoter for 3-phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, *i.e.*, Pho5, the promoters of the yeast α -mating factors, the polyhedron promoter of the baculovirus system and other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof. The nature and use of such control sequences can differ depending upon the host organism. In prokaryotes, such regulatory sequences generally include promoter, ribosomal binding site, and transcription termination sequences. The term "regulatory sequence" is intended to include, at a minimum, components whose presence can influence expression, and can also include additional components whose presence is advantageous, for example, leader sequences and fusion partner sequences. In certain embodiments, transcription of a polynucleotide sequence is under the control of a promoter sequence (or other regulatory sequence) that controls the expression of the polynucleotide in a cell-type in which expression is intended. It will also be understood that the polynucleotide can be under the control of regulatory sequences that are the same or different from those sequences which control expression of the naturally occurring form of the polynucleotide.

The term "reporter gene" refers to a nucleic acid comprising a nucleotide sequence encoding a protein that is readily detectable either by its presence or activity, including, but not limited to, luciferase, fluorescent protein (*i.e.*, green fluorescent protein), chloramphenicol acetyl transferase, β -

-48-

galactosidase, secreted placental alkaline phosphatase, β -lactamase, human growth hormone, and other secreted enzyme reporters. Generally, a reporter gene encodes a polypeptide not otherwise produced by the host cell, which is detectable by analysis of the cell(s), *i.e.*, by the direct fluorometric, radioisotopic or spectrophotometric analysis of the cell(s) and preferably without the need to kill the cells for signal analysis. In certain instances, a reporter gene encodes an enzyme, which produces a change in fluorometric properties of the host cell, which is detectable by qualitative, quantitative, or semiquantitative function or transcriptional activation. Exemplary enzymes include esterases, β -lactamase, phosphatases, peroxidases, proteases (tissue plasminogen activator or urokinase) and other enzymes whose function can be detected by appropriate chromogenic or fluorogenic substrates known to those skilled in the art or developed in the future.

The term "sequence homology" refers to the proportion of base matches between two nucleic acid sequences or the proportion of amino acid matches between two amino acid sequences. When sequence homology is expressed as a percentage, *i.e.*, 50%, the percentage denotes the proportion of matches over the length of sequence from a desired sequence (*i.e.*, SEQ. ID NO: 1) that is compared to some other sequence. Gaps (in either of the two sequences) are permitted to maximize matching; gap lengths of 15 bases or less are usually used, 6 bases or less are used more frequently, with 2 bases or less used even more frequently. The term "sequence identity" means that sequences are identical (*i.e.*, on a nucleotide-by-nucleotide basis for nucleic acids or amino acid-by-amino acid basis for polypeptides) over a window of comparison. The term "percentage of sequence identity" is calculated by comparing two optimally aligned sequences over the comparison window, determining the number of positions at which the identical amino acids occurs in both sequences to yield the number of matched positions, dividing the number of matched positions by the total number of positions in the comparison window, and multiplying the result by 100 to yield the percentage of sequence identity. Methods to calculate

-49-

sequence identity are known to those of skill in the art and described in further detail herein.

As used herein, the term "sequencing" refers to determining the ordered linear sequence of nucleotides or amino acids of a DNA, RNA, or protein target sample, using conventional manual or automated laboratory techniques.

The term "small molecule" refers to a compound, which has a molecular weight of less than about 5 kilodalton (kD), less than about 2.5 kD, less than about 1.5 kD, or less than about 0.9 kD. Small molecules can be, for example, nucleic acids, peptides, polypeptides, peptide nucleic acids, peptidomimetics, carbohydrates, lipids, or other organic (carbon containing) or inorganic molecules. The term "small organic molecule" refers to a small molecule that is often identified as being an organic or medicinal compound, and does not include molecules that are exclusively nucleic acids, peptides, or polypeptides.

The term "soluble" as used herein with reference to a polypeptide of the invention or other protein means that upon expression in cell culture, at least some portion of the polypeptide or protein expressed remains in the cytoplasmic fraction of the cell and does not fractionate with the cellular debris upon lysis and centrifugation of the lysate. Solubility of a polypeptide can be increased by a variety of art recognized methods, including fusion to a heterologous amino acid sequence, deletion of amino acid residues, amino acid substitution (*i.e.*, enriching the sequence with amino acid residues having hydrophilic side chains), and chemical modification (*i.e.*, addition of hydrophilic groups). The solubility of polypeptides can be measured using a variety of art recognized techniques, including dynamic light scattering to determine aggregation state, UV absorption, centrifugation to separate aggregated from non-aggregated material, and SDS gel electrophoresis (*i.e.*, the amount of protein in the soluble fraction is compared to the amount of protein in the soluble and insoluble fractions combined). When expressed in a host cell, the polypeptides of the invention can be at least about 1%, 2%, 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90% or more soluble, *i.e.*,

-50-

at least about 1%, 2%, 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90% or more of the total amount of protein expressed in the cell is found in the cytoplasmic fraction. In certain embodiments, a one liter culture of cells expressing a polypeptide of the invention will produce at least about 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, 30, 40, 50 milligrams or more of soluble protein. In an exemplary embodiment, a polypeptide of the invention is at least about 10% soluble and will produce at least about 1 milligram of protein from a one liter cell culture.

As used herein, the term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "specifically hybridizes" refers to detectable and specific nucleic acid binding. Polynucleotides, oligonucleotides, and nucleic acids of the invention selectively hybridize to nucleic acid strands under hybridization and wash conditions that minimize appreciable amounts of detectable binding to nonspecific nucleic acids. Stringent conditions can be used to achieve selective hybridization conditions as known in the art and discussed herein. Generally, the nucleic acid sequence homology between the polynucleotides, oligonucleotides, and nucleic acids of the invention and a nucleic acid sequence of interest will be at least 30%, 40%, 50%, 60%, 70%, 80%, 85%, 90%, 95%, 98%, 99%, or more. In certain instances, hybridization and washing conditions are performed under stringent conditions according to conventional hybridization procedures and as described further herein.

As used herein, the terms "structure coordinates", "atomic coordinates", and "structural coordinates" are used interchangeably and refer to coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without experimental error. In general, the

-51-

error in the coordinates tends to be reduced as the resolution is increased, since more experimental diffraction data is available for the model fitting and refinement. Thus, for example, more diffraction data can be collected from a crystal that diffracts to a resolution of 2.0 angstroms than from a crystal that diffracts to a lower resolution, such as 2.5 or 3.0 angstroms. Consequently, the refined structural coordinates will usually be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of ligands for a CAR polypeptide depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then the design process will be ineffective. In most cases, it is very difficult or impossible to collect sufficient diffraction data to define atomic coordinates precisely when the crystals diffract to a resolution of 3.0 angstroms or poorer. Thus, in most cases, it is difficult to use X-ray structures in structure-based ligand design when the X-ray structures are based on crystals that diffract to a resolution of only 3.0 angstroms or poorer. However, common experience has shown that crystals diffracting to 2.0-2.5 angstroms or better can yield X-ray structures with sufficient accuracy to greatly facilitate structure-based drug design. Further improvement in the resolution can further facilitate structure-based design, but the coordinates obtained at 2.0-2.5 angstroms resolution are generally considered adequate for most purposes.

Also, those of skill in the art will understand that nuclear receptors can adopt different conformations when different ligands are bound, or in the absence of any ligand. In particular, in most nuclear receptors, the AF2 helix can adopt different conformations when agonists and antagonists (or inverse agonists) are bound. More subtle conformational changes occur in other parts of the LBD when the AF2 helix is shifted. Generally, structure-based design of ligands that modulate CAR activity requires an understanding of the "activated" conformation that occurs when agonists are bound (or in the absence of ligand), as well as the "repressed" conformation that occurs when antagonists (or inverse agonists) are bound. The crystal structure of CAR bound to Compound 1 provides the "repressed" structure of CAR. In one embodiment, the "activated" conformation of CAR can be modeled

-52-

approximately by using the "repressed" CAR structure as a starting structure, and then adjusting the conformation of the residues at the C-terminal end of the structure, residues 332-348, to form an AF2 helix with conformation, position, and orientation similar to that observed in the "activated" conformations of other nuclear receptors. It should be noted that the X-ray structure of CAR bound to Compound 1, which is an inverse agonist, revealed a completely novel, unexpected conformation for the residues that normally comprise the AF2 helix and the AF2 linking segment. No conventional modeling procedure could have predicted this novel "repressed" structure from an X-ray structure of the "activated" conformation of CAR.

The terms "stringent conditions" or "stringent hybridization conditions" refer to conditions that promote specific hybridization between two complementary polynucleotide strands so as to form a duplex. Stringent conditions can be selected to be about 5°C lower than the thermal melting point (T_m) for a given polynucleotide duplex at a defined ionic strength and pH. The length of the complementary polynucleotide strands and their GC content will determine the T_m of the duplex, and thus the hybridization conditions necessary for obtaining a desired specificity of hybridization. The T_m is the temperature (under defined ionic strength and pH) at which 50% of a polynucleotide sequence hybridizes to a perfectly matched complementary strand. In certain cases it can be desirable to increase the stringency of the hybridization conditions to be about equal to the T_m for a particular duplex.

A variety of techniques for estimating the T_m are available. Typically, G-C base pairs in a duplex are estimated to contribute about 3°C to the T_m, while A-T base pairs are estimated to contribute about 2°C, up to a theoretical maximum of about 80-100°C. However, more sophisticated models of T_m are available in which G-C stacking interactions, solvent effects, the desired assay temperature and the like are taken into account. For example, probes can be designed to have a dissociation temperature (T_d) of approximately 60°C, using the formula: $T_d = (((((3 \times \#GC) + (2 \times \#AT)) \times 37) - 562) / \#bp) - 5$; where #GC, #AT, and #bp are the number of guanine-cytosine base pairs, the

-53-

number of adenine-thymine base pairs, and the number of total base pairs, respectively, involved in the formation of the duplex.

Hybridization can be carried out in 5x SSC, 4x SSC, 3x SSC, 2x SSC, 1x SSC or 0.2x SSC for at least about 1 hour, 2 hours, 5 hours, 12 hours, or 24 hours. The temperature of the hybridization can be increased to adjust the stringency of the reaction, for example, from about 25°C (room temperature), to about 45°C, 50°C, 55°C, 60°C, or 65°C. The hybridization reaction can also include another agent affecting the stringency; for example, hybridization conducted in the presence of 50% formamide increases the stringency of hybridization at a defined temperature.

The hybridization reaction can be followed by a single wash step, or two or more wash steps, which can be at the same or a different salinity and temperature. For example, the temperature of the wash can be increased to adjust the stringency from about 25°C (room temperature), to about 45°C, 50°C, 55°C, 60°C, 65°C, or higher. The wash step can be conducted in the presence of a detergent, *i.e.*, 0.1 or 0.2% SDS. For example, hybridization can be followed by two wash steps at 65°C each for about 20 minutes in 2x SSC, 0.1% SDS, and optionally two additional wash steps at 65°C each for about 20 minutes in 0.2x SSC, 0.1% SDS.

Exemplary stringent hybridization conditions include overnight hybridization at 65°C in a solution comprising, or consisting of, 50% formamide, 10x Denhardt's Solution (0.2% Ficoll, 0.2% Polyvinylpyrrolidone, 0.2% bovine serum albumin) and 200 µg/ml of denatured carrier DNA, *i.e.*, sheared salmon sperm DNA, followed by two wash steps at 65°C each for about 20 minutes in 2x SSC, 0.1% SDS, and two wash steps at 65°C each for about 20 minutes in 0.2x SSC, 0.1% SDS.

Hybridization can include hybridizing two nucleic acids in solution, or a nucleic acid in solution to a nucleic acid attached to a solid support, *i.e.*, a filter. When one nucleic acid is on a solid support, a prehybridization step can be conducted prior to hybridization. Prehybridization can be carried out for at least about 1 hour, 3 hours or 10 hours in the same solution and at the same

-54-

temperature as the hybridization solution (without the complementary polynucleotide strand).

Appropriate stringency conditions are known to those skilled in the art or can be determined experimentally by the skilled artisan. See e.g. Ausubel
5 *et al.*, 1994; Sambrook & Russell, 2001; Agrawal, 1993; Tibanyenda *et al.*, 1984; Ebel *et al.*, 1992.

The term "structural motif", when used in reference to a polypeptide, refers to a polypeptide that, although it can have different amino acid sequences, can result in a similar structure, wherein by structure is meant that
10 the motif forms generally the same tertiary structure, or that certain amino acid residues within the motif, or alternatively their backbone or side chains (which can or can not include the C α atoms of the side chains) are positioned in a like relationship with respect to one another in the motif.

As applied to proteins, the term "substantial identity" means that two
15 protein sequences, when optimally aligned, such as by the programs GAP or BESTFIT using default gap weights, typically share at least about 70 percent sequence identity, alternatively at least about 80, 85, 90, 95 percent sequence identity or more. In certain instances, residue positions that are not identical differ by conservative amino acid substitutions, which are described above.

20 As used herein, the term "substantially pure" refers to a polynucleotide or polypeptide that is substantially free of the sequences and molecules with which it is associated in its natural state, as well as from those molecules used in the isolation procedure. The term "substantially free" refers to that the sample is in one embodiment at least 50%, in another embodiment at least
25 70%, in another embodiment at least 80%, and in still another embodiment at least 90% free of the sequences and molecules with which is it associated in nature.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect
30 a modification from conditions known to be present in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length.

-55-

Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

The term "test compound" refers to a molecule to be tested by one or more screening method(s) as a putative modulator of a polypeptide of the invention or other biological entity or process. A test compound is usually not known to bind to a target of interest. The term "control test compound" refers to a compound known to bind to the target (*i.e.*, a known agonist, antagonist, partial agonist or inverse agonist). The term "test compound" does not include a chemical added as a control condition that alters the function of the target to determine signal specificity in an assay. Such control chemicals or conditions include chemicals that 1) nonspecifically or substantially disrupt protein structure (*i.e.*, denaturing agents (*i.e.*, urea or guanidinium), chaotropic agents, sulfhydryl reagents (*i.e.*, dithiothreitol and β -mercaptoethanol), and proteases), 2) generally inhibit cell metabolism (*i.e.*, mitochondrial uncouplers) and 3) non-specifically disrupt electrostatic or hydrophobic interactions of a protein (*i.e.*, high salt concentrations, or detergents at concentrations sufficient to non-specifically disrupt hydrophobic interactions). Further, the term "test compound" also does not include compounds known to be unsuitable for a therapeutic use for a particular indication due to toxicity of the subject. In certain embodiments, various predetermined concentrations of test compounds are used for screening such as 0.01 μ M, 0.1 μ M, 1.0 μ M, and 10.0 μ M. Examples of test compounds include, but are not limited to peptides, nucleic acids, carbohydrates, and small molecules. The term "novel test compound" refers to a test compound that is not in existence as of the filing date of this application. In certain assays using novel test compounds, the novel test compounds comprise at least about 50%, 75%, 85%, 90%, 95% or more of the test compounds used in the assay or in any particular trial of the assay.

The term "therapeutically effective amount" refers to that amount of a modulator, drug, or other molecule that is sufficient to effect treatment when administered to a subject in need of such treatment. The therapeutically effective amount will vary depending upon the subject and disease condition

-56-

being treated, the weight and age of the subject, the severity of the disease condition, the manner of administration and the like, which can readily be determined by one of ordinary skill in the art.

The term "transfection" means the introduction of a nucleic acid, *i.e.*, an expression vector, into a recipient cell, which in certain instances involves nucleic acid-mediated gene transfer. The term "transformation" refers to a process in which a cell's genotype is changed as a result of the cellular uptake of exogenous nucleic acid. For example, a transformed cell can express a recombinant form of a polypeptide of the invention or antisense expression can occur from the transferred gene so that the expression of a naturally occurring form of the gene is disrupted.

The term "transgene" means a nucleic acid sequence, which is partly or entirely heterologous to a transgenic animal or cell into which it is introduced, or, is homologous to an endogenous gene of the transgenic animal or cell into which it is introduced, but which is designed to be inserted, or is inserted, into the animal's genome in such a way as to alter the genome of the cell into which it is inserted (*i.e.*, it is inserted at a location which differs from that of the natural gene or its insertion results in a knockout). A transgene can include one or more regulatory sequences and any other nucleic acids, such as introns, that can be necessary for optimal expression.

The term "transgenic animal" refers to any animal, for example, a mouse, rat or other non-human mammal, a bird or an amphibian, in which one or more of the cells of the animal contain heterologous nucleic acid introduced by way of human intervention, such as by transgenic techniques well known in the art. The nucleic acid is introduced into the cell, directly or indirectly, by way of deliberate genetic manipulation, such as by microinjection or by infection with a recombinant virus. The term genetic manipulation does not include classical cross-breeding, or *in vitro* fertilization, but rather is directed to the introduction of a recombinant DNA molecule. This molecule can be integrated within a chromosome, or it can be extrachromosomally replicating DNA. In the typical transgenic animals described herein, the transgene

-57-

causes cells to express a recombinant form of a protein. However, transgenic animals in which the recombinant gene is silent are also contemplated.

As used herein, the term "unit cell" refers to a basic parallelepiped shaped block. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" refers to the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors, a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles α , β and γ define the angles between the vectors: angle α is the angle between vectors b and c; angle β is the angle between vectors a and c; and angle γ is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells, each unit cell comprising a complete representation of the unit of pattern, the repetition of which builds up the crystal.

Unless otherwise indicated, all numbers expressing quantities of ingredients, reaction conditions, and so forth used in the specification and claims are to be understood as being modified in all instances by the term "about". Accordingly, unless indicated to the contrary, the numerical parameters set forth in this specification and attached claims are approximations that can vary depending upon the desired properties sought to be obtained by the present invention.

II. Description of Tables

Table 1 is a table summarizing the crystal and data statistics obtained from the crystallized ligand-binding domain of CAR in complex with the ligand Compound 1. Data on the unit cell are presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

Table 2 is a table of the atomic coordinate data obtained from X-ray diffraction from the ligand-binding domain of CAR in complex with the ligand Compound 1.

-58-

Table 3 is a table of the atomic structure coordinate data of the poly-alanine model of the conserved vitamin D receptor ligand-binding domain.

III. General Considerations

5 The present invention is applicable *mutatis mutandis* to all CARs, as discussed herein, based in part on the patterns of CAR structure and modulation that have emerged as a consequence of determining the three dimensional structure of CAR with bound ligand. Analysis and alignment of amino acid sequences, and X-ray and NMR structure determinations, have
10 shown that nuclear receptors have a modular architecture with three main domains:

- 1) a variable amino-terminal domain;
- 2) a highly conserved DNA-binding domain (DBD); and
- 3) a less conserved carboxy-terminal ligand-binding domain (LBD).

15 In addition, nuclear receptors can have linker segments of variable length between these major domains. Sequence analysis and X-ray crystallography, including the work of the present invention, have confirmed that CARs, and indeed many NRs, also have the same general modular architecture, with the same three domains. The function of the CARs in human cells presumably
20 requires all three domains in a single amino acid sequence. However, the modularity of the CARs permits different domains of each protein to separately accomplish certain functions.

Previous analysis of the nuclear receptors has revealed multiple discrete functional modules within the family that display generalized
25 functional characteristics (for review see Beato *et al.*, 1995; Kastner *et al.*, 1995; Mangelsdorf & Evans, 1995; Tzukerman *et al.*, 1994). A variable amino-terminal domain (A/B) is present that sometimes contains a strong and autonomous activation function (AF1), shown to be critical for cell and target gene specificity (Tora *et al.*, 1988). A more carboxyl-terminal central region
30 contains a DNA binding domain (DBD) characterized by two C4-type zinc fingers. The DBD binds to specific genomic response elements and thereby regulates the transcriptional activity of select genes containing the response

-59-

elements. At the distal carboxyl terminus, a ligand-binding domain (LBD) is present containing a highly conserved second transactivation function (AF2) that is important for hormone-dependent transcriptional transactivation (Lanz & Rusconi, 1994).

5 Typically, the LBD forms a three-layered anti-parallel helical sandwich composed of 10-14 α helices and a β -sheet with 2-4 strands. The helices pack together so as to leave a binding pocket near the middle of the bundle, capped on one side by the β -sheet, and, in the "activated" state, capped on the other side by the AF2-helix. Comparison of apo, agonist-bound, and
10 antagonist-bound nuclear receptor structures has led to a model for ligand-inducible receptor action. In this model, the agonist (activating) ligands tend to hold the AF2 helix in a conformation where it "caps" the binding pocket. Antagonistic ligands usually shift the AF2 helix out of this "active" position. The AF2 helix can also shift into other conformations, positions, and
15 orientations in the absence of ligand. Constitutively active receptors such as CAR should presumably utilize a similar mechanism of action, except that the AF2 helix adopts the "active" position, capping the ligand-binding pocket, even in the absence of ligand. Inverse agonists would presumably tend to shift the AF2 helix out of this "active" position, whereas superagonists would
20 presumably tend to hold the AF2 helix more tightly in the active position. Central to the efficient ligand-induced transcriptional activation is the recruitment of co-regulator proteins – coactivators and co-repressors, which interact with the LBD and activate or repress transactivation, respectively (Moras & Gronemeyer, 1998; Weatherman *et al.*, 1999; McKenna & O'Malley,
25 2000). In general, the conformational changes described above involving the AF2 helix cause changes in the affinity of the LBD for co-repressors versus coactivators. The binding of an agonist results in a dissociation of co-repressors and brings the AF2 into a context where it can interact with transcriptional coactivators. Likewise, an antagonist would be expected to
30 disrupt the binding of coactivators.

Sequences that function in nuclear localization, receptor dimerization, and interaction with heat-shock proteins (Gronemeyer & Laudet, 1995) are

-60-

also present within the nuclear receptor substructure. Through the coordinated action of these separate functional domains, nuclear receptor activation by ligand culminates in modulation of target gene expression through DNA interactions (Tsai & O'Malley, 1994) or in certain other cases through cross-talk with other cell signaling pathways (Stein & Yang, 1995; Paech *et al.*, 1998). In short, a ligand alters nuclear receptor function by altering the conformation of the receptor and consequently the constellation of protein-protein interactions in which the receptor is engaged (Freedman, 1999).

Some of the functions of a domain within the full-length receptor are preserved when that particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques, a modular domain can sometimes be separated from the parent protein. Using conventional molecular biology techniques, each domain can usually be separately expressed with its original function intact or, as discussed herein below, chimeras comprising two different proteins can be constructed, wherein the chimeras retain the properties of the individual functional domains of the respective nuclear receptors from which the chimeras were generated.

The LBD is the second most highly conserved domain in these 3 domains. As its name suggests, the LBD binds ligands. With many nuclear receptors binding of the ligand can induce a conformational change in the LBD that can, in turn, increase or decrease transcription of certain target genes. The LBD also participates in other functions, including dimerization and nuclear translocation.

X-ray structures have shown that most nuclear receptor LBDs adopt the same general folding pattern. This fold includes 10-12 alpha helices arranged in a bundle, together with several beta-strands, additional alpha helices and linking segments. The major alpha helices and beta-strands have been numbered differently in different publications. The present disclosure follows the numbering scheme of Nolte *et al.*, 1998, where the major alpha-helices and beta-strands in PPAR γ were designated sequentially through the amino acid sequence as H1, H2, S1, H2', H3, H3', H4, H5, S2, S3, S4, H6,

-61-

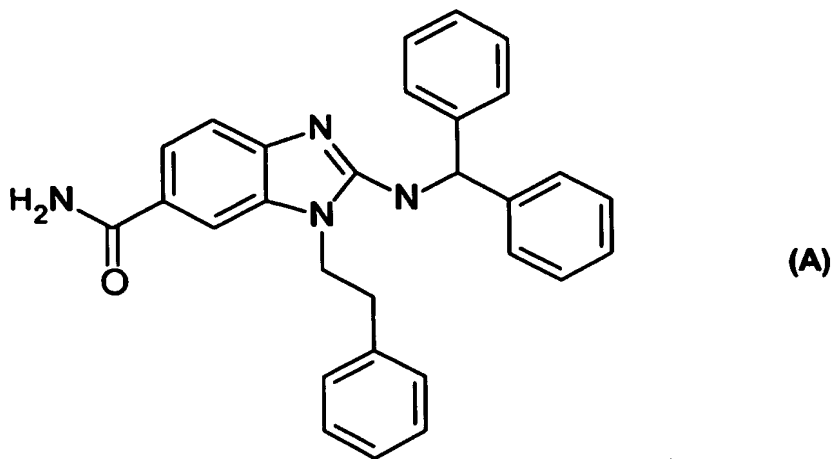
H7, H8, H9, H10 and HAF. The alpha helix at the C-terminal end, HAF, is also called "helix-AF", "helix-AF2" the "AF2 helix" or "helix-12". Most, but not all, of these alpha helices and beta-strands are observed in the structure of CAR. An additional helix, designated here as "helix-X", is observed in the structure of CAR bound to Compound 1 on the C-terminal side of H10.

As described herein, the LBD of a CAR can be expressed, crystallized, its three dimensional structure determined with a ligand bound as disclosed in the present invention, and computational methods can be used to design ligands to its LBD.

IV. Synthesis of CAR Ligands and Intermediates

IV.A. Compound 1 – An Embodiment of a Synthetic CAR Ligand

In one embodiment, the present invention provides compounds of Compound 1 (Formula (A) below) and tautomeric forms, pharmaceutically acceptable salts and solvates thereof:



IV.B. Synthesis of Compound 1 and Intermediates

Compound 1, which was co-crystallized with the CAR LBD in the present invention, can be prepared as described in Example 6 and shown in

-62-

Figure 7. Briefly, a solution of 3-fluoro-4-nitrobenzoic acid in anhydrous *N,N*-dimethylformamide was treated with [O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate] followed by *N,N*-diisopropylethylamine. After shaking for 5 minutes, the mixture was added to polystyrene Rink amide AM resin, and the reaction was rotated at 25°C for 18 hours. The reaction solution was drained, and the resin was washed with *N,N*-dimethylformamide, dichloromethane, methanol, and dichloromethane. The dried resin was treated with a 0.5 M phenethylamine in *N*-methylpyrrolidinone solution and incubated with rotation for 15 hours at 70°C. The reaction was cooled to room temperature, drained, and the resin was washed as before. The resin was then treated with a 2.0 M SnCl₂•dihydrate in *N*-methylpyrrolidinone solution for 24 hours at 25°C with rotation. The reaction was drained and the resin washed with 30% ethylenediamine, *N,N*-dimethylformamide, dichloromethane, methanol, and dichloromethane. The dried diamine resin was treated with a 0.5 M benzyhydriyl isothiocyanate in *N*-methylpyrrolidinone solution and a 1.0 M diisopropylcarbodiimide in *N*-methylpyrrolidinone solution at 80°C with rotation. After 24 hours, the reaction was cooled to 25°C, drained, and the resin was washed with *N,N*-dimethylformamide, dichloromethane, methanol, and dichloromethane. The resin was then treated with 95:5 TFA:H₂O and rotated at 25°C for 3 hours. The resin was drained and washed with dichloromethane. The filtrate was concentrated *in vacuo* to give an oil. The oil was redissolved in dichloromethane and the solution was washed twice with saturated sodium bicarbonate. The organic layer was dried (Na₂SO₄), filtered, and concentrated *in vacuo*. The crude product was triturated with Et₂O/hexanes, and the solid was collected by filtration to give Compound 1 as an off-white solid.

V. Production of CAR Polypeptides

The native and mutated CAR polypeptides, and fragments thereof, of the present invention can be chemically synthesized in whole or part using techniques that are well known in the art (see e.g., Creighton, 1983, incorporated herein in its entirety). Alternatively, methods which are well

-63-

known to those skilled in the art can be used to construct expression vectors containing a partial or the entire native or mutated CAR polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination (see e.g., the techniques described throughout Sambrook & Russell, 2001, and Ausubel *et al.*, 1994, both incorporated herein in their entirety).

A variety of host-expression vector systems can be utilized to express a CAR coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing a CAR coding sequence; yeast transformed with recombinant yeast expression vectors containing a CAR coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing a CAR coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing a CAR coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, can be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage λ , plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like can be used. When cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter can be used. When cloning in plant cell systems, promoters derived from the genome of plant cells, such as heat shock promoters; the promoter for the small subunit of ribulose biphosphate carboxylase (RUBISCO); the promoter for the chlorophyll a/b binding protein; or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) can be used. When cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein

-64-

promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) can be used.

In each of these systems, one of ordinary skill in the art will appreciate that other promoters can be used, and as such, the list presented is not intended to be exhaustive.

VI. Analysis of Protein Properties

VI.A. Analysis of Proteins by X-ray Crystallography Generally

VI.A.1. X-ray Structure Determination

Exemplary methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and, in view of this specification, variations on these methods will be apparent to those skilled in the art (see Ducruix & Geige, 1992).

A variety of methods involving X-ray crystallography are contemplated by the present invention. For example, the present invention contemplates producing a crystallized polypeptide of the invention, or a fragment thereof, by: (a) introducing into a host cell an expression vector comprising a nucleic acid encoding for a polypeptide of the invention, or a fragment thereof; (b) culturing the host cell in a cell culture medium to express the polypeptide or fragment; (c) isolating the polypeptide or fragment from the cell culture; and (d) crystallizing the polypeptide or fragment thereof. Alternatively, the present invention contemplates determining the three dimensional structure of a crystallized polypeptide of the invention, or a fragment thereof, by: (a) crystallizing a polypeptide of the invention, or a fragment thereof, such that the crystals will diffract X-rays to a resolution of 2.5 Å or better; and (b) analyzing the polypeptide or fragment by X-ray diffraction to determine the three-dimensional structure of the crystallized polypeptide.

X-ray crystallography techniques generally require that the protein molecules be available in the form of a crystal. Crystals can be grown from a solution containing a purified polypeptide of the invention, or a fragment thereof (i.e., a ligand-binding domain), by a variety of conventional processes. These processes include, for example, batch, liquid, bridge, dialysis, and

-65-

vapor diffusion (*i.e.*, hanging drop or sitting drop methods). See *e.g.*, McPherson, 1982; McPherson, 1990; Webe, 1991.

5 In certain embodiments, native crystals of the invention can be grown by adding precipitants to the concentrated solution of the polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water can be removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

10 The formation of crystals is dependent on a number of different parameters, including pH, temperature, protein concentration, the nature of the solvent and precipitant, as well as the presence of added ions or ligands to the protein. In addition, the sequence of the polypeptide being crystallized will have a significant affect on the success of obtaining crystals. Many routine crystallization experiments can be needed to screen all these
15 parameters for the few combinations that might give crystal suitable for X-ray diffraction analysis. See *e.g.*, Jancarik & Kim, 1991.

Crystallization robots can automate and speed up the work of reproducibly setting up large number of crystallization experiments. Once some suitable set of conditions for growing the crystal are found, variations of
20 the condition can be systematically screened in order to find the set of conditions which allows the growth of sufficiently large, single, well ordered crystals. In certain instances, a polypeptide of the invention is co-crystallized with a ligand: in one embodiment, Compound 1.

A number of methods are available to produce suitable radiation for X-
25 ray diffraction. For example, X-ray beams can be produced by synchrotron rings where electrons (or positrons) are accelerated through an electromagnetic field while traveling at close to the speed of light. Because the admitted wavelength can also be controlled, synchrotrons can be used as a tunable X-ray source (Hendrickson, 2000). For less conventional Laue
30 diffraction studies, polychromatic X-rays covering a broad wavelength window are used to observe many diffraction intensities simultaneously (Stoddard,

-66-

1998). Neutrons can also be used for solving protein crystal structures (Gutberlet *et al.*, 2001).

Before data collection commences, a protein crystal can be frozen to protect it from radiation damage. A number of different cryo-protectants can be used to assist in freezing the crystal, such as methyl pentanediol (MPD), isopropanol, ethylene glycol, glycerol, formate, citrate, mineral oil, or a low-molecular-weight polyethylene glycol (PEG). The present invention contemplates a composition comprising a polypeptide of the invention and a cryo-protectant. As an alternative to freezing the crystal, the crystal can also be used for diffraction experiments performed at temperatures above the freezing point of the solution. In these instances, the crystal can be protected from desiccation by placing it in a narrow capillary of a suitable material (generally glass or quartz) with some of the crystal growth solution included in order to maintain vapor pressure.

X-ray diffraction results can be recorded by a number of ways known to one of skill in the art. Examples of area electronic detectors include charge coupled device detectors, multi-wire area detectors, and phosphorimager detectors (Amemiya, 1997; Westbrook & Naday, 1997; Kahn & Fourme, 1997).

A suitable system for laboratory data collection might include a Bruker AXS Proteum R system, equipped with a copper rotating anode source, Confocal MAX-FLUXTM optics and a SMART 6000 charge coupled device detector. Collection of X-ray diffraction patterns is well known to those skilled in the art (see e.g. Ducruix & Geige, 1992).

The theory behind diffraction by a crystal upon exposure to X-rays is well known. Because phase information is not directly measured in the diffraction experiment and is needed to reconstruct the electron density map, methods that can recover this missing information are required. One method of solving structures *ab initio* is the real/reciprocal space cycling technique. Suitable real/reciprocal space cycling search programs include Shake-and-Bake (Miller *et al.*, 1993; Weeks *et al.*, 1994).

-67-

Other methods for deriving phases might also be needed. These techniques generally rely on the idea that if two or more measurements of the same reflection are made where strong, measurable, differences are attributable to the characteristics of a small subset of the atoms alone, then the contributions of other atoms can be, to a first approximation, ignored, and the positions of these atoms can be determined from the difference in scattering by one of the above techniques. Knowing the position and scattering characteristics of those atoms, one can calculate what phase the overall scattering must have had to produce the observed differences.

One version of this technique is the isomorphous replacement technique, which requires the introduction of new, well ordered, X-ray scatterers into the crystal. These additions are usually heavy metal atoms, (so that they make a significant difference in the diffraction pattern); and if the additions do not change the structure of the molecule or of the crystal cell, the resulting crystals should be isomorphous. Isomorphous replacement experiments are usually performed by diffusing different heavy-metal metals into the channels of a pre-existing protein crystal. Growing the crystal from protein that has been soaked in the heavy atom is also possible (Petsko, 1985). Alternatively, the heavy atom can also be reactive and attached covalently to exposed amino acid side chains (such as the sulfur atom of cysteine) or it can be associated through non-covalent interactions. It is sometimes possible to replace endogenous light metals in metallo-proteins with heavier ones, *i.e.*, zinc by mercury, or calcium by samarium (Petsko, 1985). Exemplary sources for such heavy compounds include, but are not limited to, sodium bromide, sodium selenate, trimethyl lead acetate, mercuric chloride, methyl mercury acetate, platinum tetracyanide, platinum tetrachloride, nickel chloride, and europium chloride.

A second technique for generating differences in scattering involves the phenomenon of anomalous scattering. X-rays that cause the displacement of an electron in an inner shell to a higher shell are subsequently rescattered, but there is a time lag that shows up as a phase delay. This phase delay is observed as a (generally quite small) difference in

-68-

intensity between reflections known as Friedel mates that would be identical if no anomalous scattering were present. A second effect related to this phenomenon is that differences in the intensity of scattering of a given atom will vary in a wavelength-dependent manner, giving rise to what are known as
5 dispersive differences. In principle, anomalous scattering occurs with all atoms, but the effect is strongest with heavy atoms, and can be maximized by using X-rays at a wavelength where the energy is equal to the difference in energy between shells. The technique therefore requires the incorporation of some heavy atom much as is needed for isomorphous replacement, although
10 for anomalous scattering a wider variety of atoms are suitable, including lighter metal atoms (copper, zinc, iron) in metallo-proteins. One method for preparing a protein for anomalous scattering involves replacing the methionine residues in whole or in part with selenium-containing selenomethionine. Soaking with halide salts such as bromides and other non-
15 reactive ions can also be effective (Dauter *et al.*, 2001).

In another process, known as multiple anomalous scattering or MAD, two to four suitable wavelengths of data are collected. (Hendrickson & Ogata, 1997). Phasing by various combinations of single and multiple isomorphous and anomalous scattering are possible too. For example, SIRAS (single
20 isomorphous replacement with anomalous scattering) utilizes both the isomorphous and anomalous differences for one derivative to derive phases. More traditionally, several different heavy atoms are soaked into different crystals to get sufficient phase information from isomorphous differences while ignoring anomalous scattering, in the technique known as multiple
25 isomorphous replacement (MIR) (Petsko, 1985).

Additional restraints on the phases can be derived from density modification techniques. These techniques use either generally known features of electron density distribution or known facts about that particular crystal to improve the phases. For example, because protein regions of the
30 crystal scatter more strongly than solvent regions, solvent flattening/flipping can be used to adjust phases to make solvent density a uniform flat value (Zhang *et al.*, 1997). If more than one molecule of the protein is present in the

-69-

asymmetric unit, the fact that the different molecules should be virtually identical can be exploited to further reduce phase error using non-crystallographic symmetry averaging (Villieux & Read, 1997). Suitable programs for performing these processes include DM and other programs of the CCP4 suite (Collaborative Computational Project, 1994) and CNX.

The unit cell dimensions, symmetry, vector amplitude and derived phase information can be used in a Fourier transform function to calculate the electron density in the unit cell, *i.e.*, to generate an experimental electron density map. This can be accomplished using programs of the CNX or CCP4 packages. The resolution is measured in Ångstrom (Å) units, and is closely related to how far apart two objects need to be before they can be reliably distinguished. The smaller this number is, the higher the resolution and therefore the greater the amount of detail that can be seen. In alternative embodiments, crystals of the invention diffract X-rays to a resolution of better than about 4.0, 3.5, 3.0, 2.5, 2.0, 1.5, 1.0, 0.5 Å, or better.

As used herein, the term "modeling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modeling" includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

Model building can be accomplished by either the crystallographer using a computer graphics program such as TURBO or O (Jones *et al.*, 1991) or, under suitable circumstances, by using a fully automated model building program, such as wARP (Perrakis *et al.*, 1999) or MAID (Levitt, 2001). This structure can be used to calculate model-derived diffraction amplitudes and phases. The model-derived and experimental diffraction amplitudes can be compared and the agreement between them can be described by a parameter referred to as R-factor. A high degree of correlation in the amplitudes corresponds to a low R-factor value, with 0.0 representing exact agreement and 0.59 representing a completely random structure. Because the R-factor can be lowered by introducing more free parameters into the model, an

-70-

unbiased, cross-correlated version of the R-factor known as the R-free gives a more objective measure of model quality. For the calculation of this parameter a subset of reflections (generally around 10%) are set aside at the beginning of the refinement and not used as part of the refinement target.

5 These reflections are then compared to those predicted by the model (Kleywegt & Brunger, 1996).

The model can be improved using computer programs that maximize the probability that the observed data was produced from the predicted model, while simultaneously optimizing the model geometry. For example, the CNX
10 program can be used for model refinement, as can the XPLOR program (Murshudov *et al.*, 1997). In order to maximize the convergence radius of refinement, simulated annealing refinement using torsion angle dynamics can be employed in order to reduce the degrees of freedom of motion of the model (Adams *et al.*, 1997). Where experimental phase information is
15 available (*i.e.*, where MAD data was collected) Hendrickson-Lattman phase probability targets can be employed. Isotropic or anisotropic domain, group or individual temperature factor refinement, can be used to model variance of the atomic position from its mean. Well-defined peaks of electron density not attributable to protein atoms are generally modeled as water molecules.
20 Water molecules can be found by manual inspection of electron density maps, or with automatic water picking routines. Additional small molecules, including ions, cofactors, buffer molecules, or substrates can be included in the model if sufficiently unambiguous electron density is observed in a map.

In general, the R-free is rarely as low as 0.15 and can be as high as
25 0.35 or greater for a reasonably well-determined protein structure. The residual difference is a consequence of approximations in the model (inadequate modeling of residual structure in the solvent, modeling atoms as isotropic Gaussian spheres, assuming all molecules are identical rather than having a set of discrete conformers, etc.) and errors in the data (Lattman,
30 1996). In refined structures at high resolution, there are usually no major errors in the orientation of individual residues, and the estimated errors in atomic positions are usually around 0.1 - 0.2 up to 0.3 Å.

-71-

The three dimensional structure of a new crystal can be modeled using molecular replacement. The term "molecular replacement" refers to a method that involves generating a preliminary model of a molecule or complex whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known within the unit cell of the unknown crystal, so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, 1985; Rossmann, 1972).

Commonly used computer software packages for molecular replacement are CNX, X-PLOR (Brunger 1992, *Nature* 355: 472-475), AMoRE (Navaza, 1994, *Acta Crystallogr.* A50:157-163), the CCP4 package, the MERLOT package (Fitzgerald, 1988) and XTALVIEW (McCree *et al.*, 1992). The quality of the model can be analyzed using a program such as PROCHECK or 3D-Profiler (Laskowski *et al.*, 1993; Luthy *et al.*, 1992; Bowie *et al.*, 1991).

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods can also be used to develop a three dimensional model from a polypeptide sequence based on the structures of known proteins. The method utilizes a computer model of a known protein, a computer representation of the amino acid sequence of the polypeptide with an unknown structure, and standard computer representations of the structures of amino acids. This method is well known to those skilled in the art (Greer, 1985; Blundell *et al.*, 1988; Knighton *et al.*, 1992). Computer programs that can be used in homology modeling are QUANTA and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc. (now part of Accelrys Inc., San Diego, California, United States of America), or MODELLER (Rockefeller University, New York, New York, United States of America). These computer programs can also be used

-72-

for computational loop modeling techniques. See also Tosatto *et al.*, 2002; Fiser *et al.*, 2000.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in QUANTA that provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler (Luthy *et al.*, 1992; Bowie *et al.*, 1991). Once any irregularities have been resolved, the entire structure can be further refined.

Other molecular modeling techniques can also be employed in accordance with this invention. See *e.g.*, Cohen *et al.*, 1990; Navia & Murcko, 1992.

Under suitable circumstances, the entire process of solving a crystal structure can be accomplished in an automated fashion by a system such as ELVES (<http://ucxray.berkeley.edu/~jamesh/elves/index.html>) with little or no user intervention.

VI.A.2. X-ray Structure

The present invention provides methods for determining some or all of the structural coordinates for amino acids of a polypeptide of the invention, or a complex thereof.

In another aspect, the present invention provides methods for identifying a druggable region of a polypeptide of the invention. For example, one such method includes: (a) obtaining crystals of a polypeptide of the invention or a fragment thereof such that the three dimensional structure of the crystallized protein can be determined to a resolution of 2.5 Å or better; (b) determining the three dimensional structure of the crystallized polypeptide or fragment using X-ray diffraction; and (c) identifying a druggable region of a polypeptide of the invention based on the three-dimensional structure of the polypeptide or fragment.

A three dimensional structure of a molecule or complex can be described by the set of atoms that best predict the observed diffraction data

-73-

(that is, which possesses a minimal R value). Files can be created for the structure that defines each atom by its chemical identity, spatial coordinates in three dimensions, root mean squared deviation from the mean observed position and fractional occupancy of the observed position.

- 5 Those of skill in the art understand that a set of structure coordinates for a protein, complex, or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates can have little affect
- 10 on overall shape. Such variations in coordinates can be generated because of mathematical manipulations of the structure coordinates. For example, structure coordinates could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion
- 15 of the structure coordinates or any combination of the above. Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little affect on
- 20 overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. It should be noted that slight variations in individual structure coordinates of a polypeptide of the invention or a complex thereof would not be expected to significantly alter the nature of
- 25 modulators that could associate with a druggable region thereof. Thus, for example, a modulator that bound to the active site of a polypeptide of the invention would also be expected to bind to or interfere with another active site whose structure coordinates define a shape that falls within the acceptable error.
- 30 A crystal structure of the present invention can be used to make a structural or computer model of the polypeptide, complex, or portion thereof. A model can represent the secondary, tertiary, and/or quaternary structure of

-74-

the polypeptide, complex, or portion. The configurations of points in space derived from structure coordinates according to the invention can be visualized as, for example, a holographic image, a stereodiagram, a model, or a computer-displayed image, and the invention thus includes such images, diagrams, or models.

VI.A.3. Structural Equivalents

Various computational analyses can be used to determine whether a molecule or the active site portion thereof is structurally equivalent with respect to its three-dimensional structure, to all or part of a structure of a polypeptide of the invention or a portion thereof.

For the purpose of this invention, any molecule or complex or portion thereof, that has a root mean square deviation of conserved residue backbone atoms (N, C α , C, O) of less than about 1.75 Å, when superimposed on the relevant backbone atoms described by the reference structure coordinates of a polypeptide of the invention, is considered "structurally equivalent" to the reference molecule. That is to say, the crystal structures of those portions of the two molecules are substantially identical, within acceptable error. Alternatively, the root mean square deviation can be less than about 1.50, 1.40, 1.25, 1.0, 0.75, 0.5 or 0.35 Å.

The term "root mean square deviation" is understood in the art and means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object.

In another aspect, the present invention provides a scalable three-dimensional configuration of points, at least a portion of said points, and preferably all of said points, derived from structural coordinates of at least a portion of a polypeptide of the invention and having a root mean square deviation from the structure coordinates of the polypeptide of the invention of less than 1.50, 1.40, 1.25, 1.0, 0.75, 0.5 or 0.35 Å. In certain embodiments, the portion of a polypeptide of the invention is 25%, 33%, 50%, 66%, 75%,

-75-

85%, 90%, or 95% or more of the amino acid residues contained in the polypeptide.

In another aspect, the present invention provides a molecule or complex including a druggable region of a polypeptide of the invention, the druggable region being defined by a set of points having a root mean square deviation of less than about 1.75 Å from the structural coordinates for points representing (a) the backbone atoms of the amino acids contained in a druggable region of a polypeptide of the invention, (b) the side chain atoms (and optionally the C α atoms) of the amino acids contained in such druggable region, or (c) all the atoms of the amino acids contained in such druggable region. In certain embodiments, only a portion of the amino acids of a druggable region can be included in the set of points, such as 25%, 33%, 50%, 66%, 75%, 85%, 90% or 95% or more of the amino acid residues contained in the druggable region. In certain embodiments, the root mean square deviation can be less than 1.50, 1.40, 1.25, 1.0, 0.75, 0.5, or 0.35 Å. In still other embodiments, instead of a druggable region, a stable domain, fragment, or structural motif is used in place of a druggable region.

VI.A.4. Machine Displays and Machine Readable Storage Media

The invention provides a machine-readable storage medium including a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of any of the molecules or complexes, or portions thereof, of this invention. In another embodiment, the graphical three-dimensional representation of such molecule, complex, or portion thereof includes the root mean square deviation of certain atoms of such molecule by a specified amount, such as the backbone atoms by less than 1.5 Å. In another embodiment, a structural equivalent of such molecule, complex, or portion thereof, can be displayed. In another embodiment, the portion can include a druggable region of the polypeptide of the invention.

According to one embodiment, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-

-76-

ray diffraction data obtained from a molecule or complex, wherein said computer includes: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of a polypeptide of the invention; (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data from said molecule or complex; (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b); (d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or complex. In certain embodiments, the structural coordinates displayed are structurally equivalent to the structural coordinates of a polypeptide of the invention.

In an alternative embodiment, the machine-readable data storage medium includes a data storage material encoded with a first set of machine readable data which includes the Fourier transform of the structure coordinates of a polypeptide of the invention or a portion thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data including the X-ray diffraction pattern of a molecule or complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, a system for reading a data storage medium can include a computer including a central processing unit (CPU), a working memory which can be, *i.e.*, random access memory (RAM) or "core" memory, mass storage memory (such as one or more disk drives or CD-ROM drives), one or more display devices (*i.e.*, cathode-ray tube ("CRT") displays, light emitting diode (LED) displays, liquid crystal displays (LCDs), electroluminescent displays, vacuum fluorescent displays, field emission displays (FEDs), plasma

-77-

displays, projection panels, etc.), one or more user input devices (*i.e.*, keyboards, microphones, mice, touch screens, etc.), one or more input lines, and one or more output lines, all of which are interconnected by a conventional bidirectional system bus. The system can be a stand-alone
5 computer, or can be networked (*i.e.*, through local area networks, wide area networks, intranets, extranets, or the internet) to other systems (*i.e.*, computers, hosts, servers, etc.). The system can also include additional computer controlled devices such as consumer electronics and appliances.

Input hardware can be coupled to the computer by input lines and can
10 be implemented in a variety of ways. Machine-readable data of this invention can be inputted via the use of a modem or modems connected by a telephone line or dedicated data line. Alternatively or additionally, the input hardware can include CD-ROM drives or disk drives. In conjunction with a display terminal, a keyboard can also be used as an input device.

15 Output hardware can be coupled to the computer by output lines and can similarly be implemented by conventional devices. By way of example, the output hardware can include a display device for displaying a graphical representation of an active site of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer,
20 so that hard copy output can be produced, or a disk drive, to store system output for later use.

In operation, a CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage devices, accesses to and from working memory, and determines the sequence of data processing
25 steps. A number of programs can be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. References to components of the hardware system are included as appropriate throughout the following description of the data storage medium.

30 Machine-readable storage devices useful in the present invention include, but are not limited to, magnetic devices, electrical devices, optical devices, and combinations thereof. Examples of such data storage devices

-78-

include, but are not limited to, hard disk devices, CD devices, digital video disk devices, floppy disk devices, removable hard disk devices, magneto-optic disk devices, magnetic tape devices, flash memory devices, bubble memory devices, holographic storage devices, and any other mass storage peripheral
5 device. It should be understood that these storage devices include necessary hardware (*i.e.*, drives, controllers, power supplies, etc.) as well as any necessary media (*i.e.*, disks, flash cards, etc.) to enable the storage of data.

In one embodiment, the present invention contemplates a computer readable storage medium comprising structural data, wherein the data include
10 the identity and three-dimensional coordinates of a polypeptide of the invention or portion thereof. In another aspect, the present invention contemplates a database comprising the identity and three-dimensional coordinates of a polypeptide of the invention or a portion thereof. Alternatively, the present invention contemplates a database comprising a
15 portion or all of the atomic coordinates of a polypeptide of the invention or portion thereof.

VI.A.5. Structurally Similar Molecules and Complexes

Structural coordinates for a polypeptide of the invention can be used to
20 aid in obtaining structural information about another molecule or complex. This method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes that contain one or more structural features that are similar to structural features of a polypeptide of the invention. Similar structural features can include, for
25 example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged secondary structural elements (*i.e.*, α helices and β sheets). Many of the methods described above for determining the structure of a polypeptide of the invention can be used for this purpose as well.

30 For the present invention, a "structural homolog" is a polypeptide that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to the amino acid sequence of SEQ ID NOs: 2

-79-

or 4 or other polypeptide of the invention, but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit at least a portion of the tertiary (three-dimensional) structure of the polypeptide encoded by SEQ ID NOs: 2 or 4 or such other polypeptide of the invention. For example, 5 structurally homologous molecules can contain deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. Structurally homologous molecules also include modified polypeptide molecules that have been chemically or enzymatically derivatized at one or more constituent amino acids, including side chain modifications, 10 backbone modifications, and N- and C-terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and the like.

By using molecular replacement, all or part of the structure coordinates of a polypeptide of the invention can be used to determine the structure of a 15 crystallized molecule or complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*. For example, in one embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or complex whose structure is unknown including: (a) crystallizing the molecule 20 or complex of unknown structure; (b) generating an X-ray diffraction pattern from said crystallized molecule or complex; and (c) applying at least a portion of the structure coordinates for a polypeptide of the invention to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or complex whose structure is unknown.

25 In another aspect, the present invention provides a method for generating a preliminary model of a molecule or complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of a polypeptide of the invention within the unit cell of the crystal of the unknown molecule or complex so as best to account for the observed X-ray diffraction 30 pattern of the crystal of the molecule or complex whose structure is unknown.

Structural information about a portion of any crystallized molecule or complex that is sufficiently structurally similar to a portion of a polypeptide of

-80-

the invention can be resolved by this method. In addition to a molecule that shares one or more structural features with a polypeptide of the invention, a molecule that has similar bioactivity, such as the same catalytic activity, substrate specificity or ligand-binding activity as a polypeptide of the invention, can also be sufficiently structurally similar to a polypeptide of the invention to permit use of the structure coordinates for a polypeptide of the invention to solve its crystal structure.

In another aspect, the method of molecular replacement is utilized to obtain structural information about a complex containing a polypeptide of the invention, such as a complex between a modulator and a polypeptide of the invention (or a domain, fragment, ortholog, homolog etc. thereof). In certain instances, the complex includes a polypeptide of the invention (or a domain, fragment, ortholog, homolog etc. thereof) co-complexed with a modulator. For example, in one embodiment, the present invention contemplates a method for making a crystallized complex comprising a polypeptide of the invention, or a fragment thereof, and a compound having a molecular weight of less than 5 kDa, the method comprising: (a) crystallizing a polypeptide of the invention such that the crystals will diffract X-rays to a resolution of 2.5 Å or better; and (b) soaking the crystal in a solution comprising the compound having a molecular weight of less than 5 kDa, thereby producing a crystallized complex comprising the polypeptide and the compound.

Using homology modeling, a computer model of a structural homolog or other polypeptide can be built or refined without crystallizing the molecule. For example, in another aspect, the present invention provides a computer-assisted method for homology modeling a structural homolog of a polypeptide of the invention including: aligning the amino acid sequence of a known or suspected structural homolog with the amino acid sequence of a polypeptide of the invention and incorporating the sequence of the homolog into a model of a polypeptide of the invention derived from atomic structure coordinates to yield a preliminary model of the homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions

-81-

of the energy minimized model where stereochemistry restraints are violated to yield a final model of the homolog.

In another embodiment, the present invention contemplates a method for determining the crystal structure of a homolog of a polypeptide having
5 SEQ ID NO: 2 or SEQ ID NO: 4, or equivalent thereof, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof; (b)
obtaining crystals of a homologous polypeptide comprising an amino acid sequence that is at least 80% identical to the amino acid sequence set forth in
10 SEQ ID NO: 2 or SEQ ID NO: 4 such that the three dimensional structure of the crystallized homologous polypeptide can be determined to a resolution of 2.5 Å or better; and (c) determining the three dimensional structure of the crystallized homologous polypeptide by X-ray crystallography based on the atomic coordinates of the three dimensional structure provided in step (a). In
15 certain instances of the foregoing method, the atomic coordinates for the homologous polypeptide have a root mean square deviation from the backbone atoms of the polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof, of not more than 1.5 Å for all backbone atoms shared in common with the homologous polypeptide and the polypeptide having SEQ ID
20 NO: 2 or SEQ ID NO: 4, or a fragment thereof.

In another aspect, the present invention provides a method for building a model for the activated conformation of CAR, using the repressed structure of Table 2 as a template. In one embodiment, the method comprises: (a)
taking the coordinates for residues 107 to 332 directly from Table 2,
25 effectively assuming that the conformation of this portion of CAR is similar or identical in the activated and repressed states; (b) rotating and translating an X-ray structure of VDR, the Vitamin-D receptor, so as to superimpose its core backbone atoms onto corresponding atoms from CAR; (c) combining the superimposed VDR AF2 helix, residues 416-423, with residues 107-332 from
30 the initial CAR model of step (a), to serve as the starting model for residues 107-332 and 341-348 of the CAR protein in the activated conformation; (d) computationally mutating Val418, Leu419, Val421, Phe422 and Gly423 in the

-82-

transplanted VDR AF2 helix to the corresponding amino acid types in the CAR AF2 helix, which are Leu343, Gln344, Ile346, Cys347 and Ser348, respectively; and (e) adjusting the conformations of the mutated amino acid side-chains in the AF2 helix of the CAR model, residues 343, 344, and 346-348, to avoid overlaps by using either manual manipulation within molecular graphics programs or conformational search and energy minimization. In one embodiment, the method further comprises modeling the CAR AF2 linker region, residues 333-340, by using a computational loop modeling technique, recognizing that the calculated linker conformation would probably deviate considerably from the actual linker conformation.

VII. Formation of CAR Ligand-Binding Domain-Ligand Crystals

The present invention provides crystals of CAR LBD in complex with the ligand. The crystals were obtained using the methodology disclosed in the Examples. The CAR LBD-ligand crystals, which can be native or derivative crystals, have orthorhombic unit cells (an orthorhombic unit cell is a unit cell wherein $a \neq b \neq c$, and wherein $\alpha = \beta = \gamma = 90^\circ$) and space group symmetry $P2_12_12_1$. There are four CAR LBD molecules in the asymmetric unit. In this CAR crystalline form, the unit cell has dimensions of $a = 83.0 \text{ \AA}$, $b = 116.8 \text{ \AA}$, $c = 131.9 \text{ \AA}$, and $\alpha = \beta = \gamma = 90^\circ$. This crystal form can be formed in a crystallization reservoir comprising 1 \mu l of the protein-ligand solutions disclosed herein, and 1 \mu l of well buffer (e.g. 100-400 mM sodium potassium tartrate, pH 7.1-7.4).

The native and derivative co-crystals comprising a CAR LBD and a ligand disclosed in the present invention can be obtained by a variety of techniques, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g., McPherson, 1982; McPherson, 1990; Weber, 1991). In one embodiment, the vapor diffusion and hanging drop methods are used for the crystallization of CAR polypeptides and fragments thereof.

Native crystals of the present invention can be grown by dissolving a substantially pure CAR polypeptide or a fragment thereof, and optionally a

-83-

ligand, in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

5 In one embodiment of the invention, native crystals are grown by vapor diffusion (*See e.g.*, McPherson, 1982; McPherson, 1990). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 25 μ L of CAR polypeptide
10 solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand until crystals grow. Crystals generally form within two to six weeks, and are
15 suitable for data collection within approximately seven to ten weeks. Of course, those of skill in the art will recognize that the above-described crystallization procedures and conditions can be varied.

VIII. Solving a Crystal Structure of the Present Invention

20 Crystal structures of the present invention can be solved using a variety of techniques including, but not limited to isomorphous replacement, anomalous scattering, or molecular replacement methods. Computer software packages can also be used to solve a crystal structure of the present invention. Applicable software packages include, but are not limited to X-
25 PLOR™ program (Brünger, 1992; available from Accelrys Inc, San Diego, California, United States of America), Xtal View (McRee, 1992; available from the San Diego Supercomputer Center, San Diego, California, United States of America); SHELXS 97 (Sheldrick, 1990; available from the Institute of Inorganic Chemistry, Georg-August-Universität, Göttingen, Germany); HEAVY
30 (Terwilliger, Los Alamos National Laboratory) and SHAKE-AND-BAKE (Hauptman, 1997; Weeks *et al.*, 1993; available from the Hauptman-

-84-

Woodward Medical Research Institute, Buffalo, New York, United States of America). See also, Ducruix & Geige, 1992, and references cited therein.

IX. The Overall Structure of CAR α in Complex With a Ligand

5 The structure of the LBD of CAR bound with Compound 1 has been determined to 2.15Å. The statistics of the data and the refined structure are summarized in Table 1.

Table 1

10

Statistics of Crystallographic Data and Structure

Crystals	CAR/ with Compound 1
Space group	P2 ₁ 2 ₁ 2 ₁
Resolution (Å)	40.0- 2.15
Unique reflections	69,338
Completeness (%)	99.6
I/ σ (last shell)	21.7 (3.1)
R _{sym} ^a (%)	9.1
Refinement statistics	
R factor ^b (%)	21.5
R free (%)	25.1
R.M.S.D.	
bond lengths (Å)	0.007
R.M.S.D.	
bond angles(degrees)	1.308
Total non-hydrogen atoms	8601

R.M.S.D. is the root mean square deviation from ideal geometry.

$$^a R_{\text{sym}} = \sum |I_{\text{avg}} - I| / \sum I$$

^bR_{factor} = $\sum |F_P - F_{P\text{calc}}| / \sum F_P$, where F_P and F_{Pcalc} are observed and calculated structure factors, R_{free} is calculated from a randomly chosen 10% of reflections that were never used in refinement and R_{factor} is calculated for the remaining 90% of reflections.

15

-85-

In its complex with Compound 1, an inverse agonist, the CAR LBD has a structure with approximately 11 alpha helices and a beta-sheet with 3 strands, as shown in Figure 1. The CAR LBD amino acid sequence is more similar to PXR and VDR than to any other NR LBD sequence, with 50% identity to PXR and 40% identity to VDR in a core region corresponding to VDR residues 126-142, 227-289, 293-300, 302-404 and 416-421. Slightly lower percent identities are obtained by considering the entire LBD sequences; however, these percent identities are complicated by the presence of additional amino acids inserted between Helix-1 and Helix-3 in PXR.

Figure 2 gives an alignment of the human, mouse, and rat CAR sequences with the human PXR and CAR sequences, with annotation and shading to indicate structural features identified from the X-ray structures. The AF2 helix that is normally present in NR LBDs was absent in this structure, but another helix, designated here as "helix-X", was present. Helix-X includes Leu336, Ser337, Ala338, and Met339, which lie between helix-10 and the residues that normally form the AF2 helix. The hydrogen bonding pattern in helix-X is closer to that of a 3-10 helix rather than an ideal alpha helix. The absence of the AF2 helix was initially very surprising, since the amino acid sequence at the C-terminal end of CAR is very similar to the corresponding segments in VDR and PXR (Figure 2), where the AF2 helix has been seen in all available X-ray structures. Normally, activation of gene transcription depends on the binding of a coactivator, such as CREB binding protein (CBP) or steroid receptor coactivator-1 (SRC-1), and this in turn normally requires the presence of the AF2 helix in its active position. Thus, one would expect the AF2 helix to be present and in the active position in the unliganded, constitutively active form of CAR.

An inverse agonist such as Compound 1 or an antagonist could reduce gene transcription by shifting the AF2 helix into an alternative position, as has been observed with estrogen receptor (ER) bound to antagonists such as tamoxifen and raloxifene (Shiau *et al.*, 1998). Alternatively, an inverse agonist

-86-

or antagonist could act by unwinding the AF2 helix without necessarily moving it from its active position. Further analysis of the CAR X-ray structure suggests that helix-X interferes with the formation of the AF2 helix. Also, side-chains from Met339 and Met340, in and adjacent to helix-X, make
5 extensive interactions with Compound 1. This suggests that Compound 1 induces the formation of helix-X, which in turn unwinds the AF2 helix, thereby preventing coactivator binding and shutting down gene transcription.

More generally, the analysis of the X-ray structure suggests that CAR exists in equilibrium with at least two major conformations. One conformation
10 is an "activated conformation", not yet observed by X-ray crystallography, where the AF2 helix is properly formed and resides in its active position. The second major conformation is an inactivated conformation, exemplified by the complex of CAR with Compound 1, where helix-X is present and the AF2 helix is absent. While the inventors do not wish to be bound by any particular
15 hypothesized mechanism of action, it appears that, in the absence of ligand, CAR exists predominantly in the activated conformation. Agonist and "superagonist" compounds would tend to shift the equilibrium even farther towards this activated form, effectively increasing the fraction of the CAR receptor in the activated state to a level higher than that observed in the
20 absence of ligand. Inverse agonists, such as Compound 1, would act by shifting the equilibrium towards the inactivated conformation, effectively decreasing the fraction of the CAR receptor in the activated state.

The structure of CAR revealed a number of other major structural differences when compared with the structures of PXR and VDR. The CAR
25 X-ray structure allowed an accurate alignment of helix-1, confirming that PXR and VDR have 45 and 51 additional residues, respectively, in the region between helix-1 and helix-3. The conformation of this insert is unknown in VDR, as the available X-ray structures were determined with a construct where this insert was deleted. The full insert was present in the construct
30 used for the PXR X-ray structure, and most of the insert was visible in the electron density. Surprisingly, in PXR, a segment from this insert acts to displace helix-6 from its usual position where it covers the ligand-binding

-87-

pocket. This segment adopts an extended conformation that occupies less volume than helix-6, effectively opening up additional volume for the ligand in the PXR ligand-binding pocket. While the inventors do not wish to be bound by any particular hypothesized mechanism of action, based on the PXR X-ray structure and the similarity of the CAR amino acid sequence to PXR, one might expect that helix-6 would be absent or displaced away from the ligand-binding pocket, and that the ligand-binding pocket would be similarly voluminous. However, the X-ray structure of CAR reveals that helix-6 is present in CAR, and located in a position similar to that in VDR where it serves as one wall for the ligand-binding pocket. This reduces the volume available to the ligand in the ligand-binding pocket, and changes the shape of the pocket substantially. The pocket volume was calculated with the GRASP program using the atomic radii of Bondi, 1964, using a procedure where the MVP program is used to close channels to the external solvent. With this procedure, the CAR pocket has a volume of 824 Å³, similar to that of VDR, which has a volume of 871 Å³ when bound to Vitamin D, but much smaller than PXR, which has a volume of 1150-1544 Å³, depending on the ligand complexed to the protein.

The structure of the LBD of CAR comprises 11 main alpha helices, a beta sheet with 4 strands, and additional irregular structure and shorter helices. The key features are shown in Figure 1. Helices 3, 5, 6, 7, and 10 and beta strands 2, 3, and 4 enclose the ligand-binding pocket, like a three-layer sandwich (Figure 6). Helix 6, which is absent or displaced in PXR, is intact in CAR, and located in a position similar to that in VDR where it serves as part of the wall of the ligand-binding site. The structure-based sequence alignment of Figure 2 shows the secondary structures of CAR, PXR, and VDR. The presence of helix 6 in CAR reduces the size of the ligand-binding site. The limited binding pocket gives more selectivity in ligand-binding in CAR than in PXR. Binding of the antagonist in CAR causes the AF2 helix to unwind. Instead, a short sequence of amino acids located between helix 10 and the AF2 helix (Leu336, Ser337, Ala338, Met339) form a short 3-10 helix. The side chains of Leu336 and Met339, from the 3-10 helix, and Met340 form

-88-

a wall that nicely fits the side of the phenyl ring of the ligand (Figure 1 & 3). This 3-10 helix is referred to as helix X. Steric hindrance from helix X appears to contribute to the unwinding of AF2 helix

The ligand-binding site can be divided into two chambers (Figure 5).

5 One chamber contains the phenylethyl and benzimidazole-6-carboxamide fragments of the ligand. It is completely shielded from solvent. The other chamber contains the benzhydryl fragment of the ligand. This chamber is exposed to the solvent. The amino linker of the ligand is near the interface of the two chambers.

10 Figure 3 and 4 shows that the ligand fits nicely into the hydrophobic pocket of the LBD site formed mostly by aromatic or hydrophobic residues. They are Phe132, Phe161, Ile164, Asn165, Thr166, Met168, Val169, Ala198, Val199, Cys202, His203, Leu206, Phe217, Tyr224, Thr225, Ile226, Glu227, Asp228, Gly229, Ala230, Phe234, Phe238, Leu239, Leu242, Phe243, His246,
15 Tyr326, Ile330, Leu336, Ser337, Met339, and Met340.

As shown in Figure 3 and 4, there are four hydrogen bonds between the ligand and LBD. The benzimidazol-6-carboxamide forms hydrogen bonds with the carbonyl oxygen of Thr225 and Gly229 amide, respectively. The unsubstituted nitrogen on the benzimidazole forms a hydrogen bond with the
20 hydroxyl group of Tyr326. The amino group linked to the benzhydryl forms a hydrogen bond with the carboxyl oxygen of Asn165. The later two hydrogen bonds are located near the intersection of the two chambers.

X. Rational Drug Design

25 X.A. Generally

Modulators to polypeptides of the invention and other structurally related molecules, and complexes containing the same, can be identified and developed as set forth below and otherwise using techniques and methods known to those of skill in the art.

30 The present invention contemplates making any molecule that is shown to modulate the activity of a polypeptide of the invention.

-89-

In another embodiment, inhibitors, modulators of the subject polypeptides, or biological complexes containing them, can be used in the manufacture of a medicament for any number of uses, including, for example, treating any disease or other treatable condition of a patient (including
5 humans and animals), and particularly a disease caused by aberrant CAR regulation or activity.

A number of techniques can be used to screen, identify, select, and design chemical entities capable of associating with polypeptides of the invention, structurally homologous molecules, and other molecules.
10 Knowledge of the structure for a polypeptide of the invention, determined in accordance with the methods described herein, permits the design and/or identification of molecules and/or other modulators which have a shape complementary to the conformation of a polypeptide of the invention, or more particularly, a druggable region thereof. It is understood that such techniques
15 and methods can use, in addition to the exact structural coordinates and other information for a polypeptide of the invention, structural equivalents thereof described above (including, for example, those structural coordinates that are derived from the structural coordinates of amino acids contained in a druggable region as described above).

20 The term "chemical entity", as used herein, refers to chemical compounds, complexes of two or more chemical compounds, and fragments of such compounds or complexes. In certain instances, it is desirable to use chemical entities exhibiting a wide range of structural and functional diversity, such as compounds exhibiting different shapes (*i.e.*, flat aromatic rings(s),
25 puckered aliphatic rings(s), straight and branched chain aliphatics with single, double, or triple bonds) and diverse functional groups (*i.e.*, carboxylic acids, esters, ethers, amines, aldehydes, ketones, and various heterocyclic rings).

In one aspect, the method of drug design generally includes computationally evaluating the potential of a selected chemical entity to
30 associate with any of the molecules or complexes of the present invention (or portions thereof). For example, this method can include the steps of (a) employing computational means to perform a fitting operation between the

-90-

selected chemical entity and a druggable region of the molecule or complex; and (b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the druggable region.

A chemical entity can be examined either through visual inspection or
5 through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK (Dunbrack *et al.*, 1997). This procedure can include computer fitting of chemical entities to a target to ascertain how well the shape and the chemical structure of each chemical entity will complement or interfere with the structure of the subject polypeptide (Bugg *et al.*, 1993;
10 West *et al.*, 1995). Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the chemical entity to a druggable region, for example. Generally, the tighter the fit (*i.e.*, the lower the steric hindrance, and/or the greater the attractive force) the more potent the chemical entity will be because these properties are consistent with a tighter
15 binding constant. Furthermore, the more specificity in the design of a chemical entity the more likely that the chemical entity will not interfere with related proteins, which can minimize potential side-effects due to unwanted interactions.

A variety of computational methods for molecular design, in which the
20 steric and electronic properties of druggable regions are used to guide the design of chemical entities, are known. See *e.g.*, Cohen *et al.*, 1990; Kuntz *et al.*, 1982; DesJarlais, 1988; Bartlett *et al.*, 1989; Goodford *et al.*, 1985; DesJarlais *et al.*, 1986. Directed methods generally fall into two categories: (1) design by analogy in which 3-D structures of known chemical entities
25 (such as from a crystallographic database) are docked to the druggable region and scored for goodness-of-fit; and (2) de novo design, in which the chemical entity is constructed piece-wise in the druggable region. The chemical entity can be screened as part of a library or a database of molecules. Databases which can be used include ACD (MDL Systems Inc.,
30 San Leandro, California, United States of America), NCI (National Cancer Institute, Bethesda, Maryland, United States of America), CCDC (Cambridge Crystallographic Data Center, Cambridge, England, United Kingdom), CAST

-91-

(Chemical Abstract Service), Derwent (Derwent Information Limited, London, England, United Kingdom), Maybridge (Maybridge Chemical Company Ltd., Cornwall, England, United Kingdom), Aldrich (Aldrich Chemical Company, St. Louis, Missouri, United States of America), DOCK (University of California in
5 San Francisco, San Francisco, California, United States of America), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Inc., St. Louis, Missouri, United States of America) or DB-Converter (Molecular Simulations Limited, Cambridge, England, United
10 Kingdom) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

Chemical entities can be tested for their capacity to fit spatially with a druggable region or other portion of a target protein. As used herein, the term "fits spatially" means that the three-dimensional structure of the chemical entity is accommodated geometrically by a druggable region. A favorable
15 geometric fit occurs when the surface area of the chemical entity is in close proximity with the surface area of the druggable region without forming unfavorable interactions. A favorable complementary interaction occurs where the chemical entity interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating and accepting forces. Unfavorable interactions can be
20 steric hindrance between atoms in the chemical entity and atoms in the druggable region.

If a model of the present invention is a computer model, the chemical entities can be positioned in a druggable region through computational docking. If, on the other hand, the model of the present invention is a
25 structural model, the chemical entities can be positioned in the druggable region by, for example, manual docking. As used herein the term "docking" refers to a process of placing a chemical entity in close proximity with a druggable region, or a process of finding low energy conformations of a chemical entity/druggable region complex.

30 In an illustrative embodiment, the design of potential modulator begins from the general perspective of shape complimentary for the druggable region of a polypeptide of the invention, and a search algorithm is employed which is

-92-

capable of scanning a database of small molecules of known three-dimensional structure for chemical entities which fit geometrically with the target druggable region. Most algorithms of this type provide a method for finding a wide assortment of chemical entities that are complementary to the shape of a druggable region of the subject polypeptide. Each of a set of chemical entities from a particular data-base, such as the Cambridge Crystallographic Data Bank (CCDB) (Allen *et al.*, 1973), is individually docked to the druggable region of a polypeptide of the invention in a number of geometrically permissible orientations with use of a docking algorithm. In certain embodiments, a set of computer algorithms called DOCK, can be used to characterize the shape of invaginations and grooves that form the active sites and recognition surfaces of the druggable region (Kuntz *et al.*, 1982). The program can also search a database of small molecules for templates whose shapes are complementary to particular binding sites of a polypeptide of the invention (DesJarlais *et al.*, 1988).

The orientations are evaluated for goodness-of-fit and the best are kept for further examination using molecular mechanics programs, such as AMBER or CHARMM. Such algorithms have previously proven successful in finding a variety of chemical entities that are complementary in shape to a druggable region.

Goodford *et al.*, 1985 and Boobbyer *et al.*, 1989 have produced a computer program (GRID) that seeks to determine regions of high affinity for different chemical groups (termed probes) of the druggable region. GRID hence provides a tool for suggesting modifications to known chemical entities that might enhance binding. It can be anticipated that some of the sites discerned by GRID as regions of high affinity correspond to "pharmacophoric patterns" determined inferentially from a series of known ligands. As used herein, a "pharmacophoric pattern" is a geometric arrangement of features of chemical entities that is believed to be important for binding. Attempts have been made to use pharmacophoric patterns as a search screen for novel ligands (Jakes *et al.*, 1987; Brint & Willett, 1987; Jakes *et al.*, 1986).

-93-

Yet a further embodiment of the present invention utilizes a computer algorithm such as CLIX which searches such databases as CCDB for chemical entities which can be oriented with the druggable region in a way that is both sterically acceptable and has a high likelihood of achieving favorable chemical interactions between the chemical entity and the surrounding amino acid residues. The method is based on characterizing the region in terms of an ensemble of favorable binding positions for different chemical groups and then searching for orientations of the chemical entities that cause maximum spatial coincidence of individual candidate chemical groups with members of the ensemble. The algorithmic details of CLIX are described in Lawrence *et al.*, 1992.

In this way, the efficiency with which a chemical entity can bind to or interfere with a druggable region can be tested and optimized by computational evaluation. For example, for a favorable association with a druggable region, a chemical entity must preferably demonstrate a relatively small difference in energy between its bound and free states (*i.e.*, a small deformation energy of binding). Thus, certain, more desirable chemical entities will be designed with a deformation energy of binding of not greater than about 10 kcal/mole, and more preferably, not greater than 7 kcal/mole. Chemical entities can interact with a druggable region in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the chemical entity binds to the target.

In this way, the present invention provides computer-assisted methods for identifying or designing a potential modulator of the activity of a polypeptide of the invention including: supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex including at least a portion of a druggable region from a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or complex, wherein

-94-

binding to the molecule or complex is indicative of potential modulation of the activity of a polypeptide of the invention.

In another aspect, the present invention provides a computer-assisted method for identifying or designing a potential modulator to a polypeptide of the invention, supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex including at least a portion of a druggable region of a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity, and determining whether the modified chemical entity is expected to bind to the molecule or complex, wherein binding to the molecule or complex is indicative of potential modulation of the polypeptide of the invention.

In one embodiment, a potential modulator can be obtained by screening a peptide library (Scott & Smith, 1990; Cwirla *et al.*, 1990; Devlin *et al.*, 1990). A potential modulator selected in this manner could then be systematically modified by computer modeling programs until one or more promising potential drugs are identified. Such analysis has been shown to be effective in the development of HIV protease inhibitors (Lam *et al.*, 1994; Wlodawer *et al.*, 1993; Appelt, 1993; Erickson, 1993). Alternatively a potential modulator can be selected from a library of chemicals such as those that can be licensed from third parties, such as chemical and pharmaceutical companies. A third alternative is to synthesize the potential modulator de novo.

For example, in certain embodiments, the present invention provides a method for making a potential modulator for a polypeptide of the invention, the method including synthesizing a chemical entity or a molecule containing the chemical entity to yield a potential modulator of a polypeptide of the invention, the chemical entity having been identified during a computer-assisted process including supplying a computer modeling application with a set of structure

-95-

coordinates of a molecule or complex, the molecule or complex including at least one druggable region from a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to
5 bind to the molecule or complex at the active site, wherein binding to the molecule or complex is indicative of potential modulation. This method can further include the steps of evaluating the potential binding interactions between the chemical entity and the active site of the molecule or molecular complex and structurally modifying the chemical entity to yield a set of
10 structure coordinates for a modified chemical entity, which steps can be repeated one or more times.

Once a potential modulator is identified, it can then be tested in any standard assay for the macromolecule depending of course on the macromolecule, including in high throughput assays. Further refinements to
15 the structure of the modulator will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular screening assay, in particular further structural analysis by *i.e.*, ¹⁵N NMR relaxation rate determinations or X-ray crystallography with the modulator bound to the subject polypeptide. These studies can be performed
20 in conjunction with biochemical assays.

Once identified, a potential modulator can be used as a model structure, and analogs to the compound can be obtained. The analogs are then screened for their ability to bind the subject polypeptide. An analog of the potential modulator might be chosen as a modulator when it binds to the
25 subject polypeptide with a higher binding affinity than the predecessor modulator.

In a related approach, iterative drug design is used to identify modulators of a target protein. Iterative drug design is a method for optimizing associations between a protein and a modulator by determining
30 and evaluating the three dimensional structures of successive sets of protein/modulator complexes. In iterative drug design, crystals of a series of protein/modulator complexes are obtained and then the three-dimensional

-96-

structures of each complex is solved. Such an approach provides insight into the association between the proteins and modulators of each complex. For example, this approach can be accomplished by selecting modulators with inhibitory activity, obtaining crystals of this new protein/modulator complex, solving the three dimensional structure of the complex, and comparing the associations between the new protein/modulator complex and previously solved protein/modulator complexes. By observing how changes in the modulator affected the protein/modulator associations, these associations can be optimized.

In addition to designing and/or identifying a chemical entity to associate with a druggable region, as described above, the same techniques and methods can be used to design and/or identify chemical entities that either associate, or do not associate, with affinity regions, selectivity regions or undesired regions of protein targets. By such methods, selectivity for one or a few targets, or alternatively for multiple targets, from the same species or from multiple species, can be achieved.

For example, a chemical entity can be designed and/or identified for which the binding energy for one druggable region, *i.e.*, an affinity region or selectivity region, is more favorable than that for another region, *i.e.*, an undesired region, by about 20%, 30%, 50% to about 60% or more. It can be the case that the difference is observed between (a) more than two regions, (b) between different regions (selectivity, affinity or undesirable) from the same target, (c) between regions of different targets, (d) between regions of homologs from different species, or (e) between other combinations. Alternatively, the comparison can be made by reference to the K_d , usually the apparent K_d , of said chemical entity with the two or more regions in question.

In another aspect, prospective modulators are screened for binding to two nearby druggable regions on a target protein. For example, a modulator that binds a first region of a target polypeptide does not bind a second nearby region. Binding to the second region can be determined by monitoring changes in a different set of amide chemical shifts in either the original screen or a second screen conducted in the presence of a modulator (or potential

-97-

modulator) for the first region. From an analysis of the chemical shift changes, the approximate location of a potential modulator for the second region is identified. Optimization of the second modulator for binding to the region is then carried out by screening structurally related compounds (*i.e.*,
5 analogs as described above).

When modulators for the first region and the second region are identified, their location and orientation in the ternary complex can be determined experimentally. On the basis of this structural information, a linked compound, *i.e.*, a consolidated modulator, is synthesized in which the
10 modulator for the first region and the modulator for the second region are linked. In certain embodiments, the two modulators are covalently linked to form a consolidated modulator. This consolidated modulator can be tested to determine if it has a higher binding affinity for the target than either of the two individual modulators. A consolidated modulator is selected as a modulator
15 when it has a higher binding affinity for the target than either of the two modulators. Larger consolidated modulators can be constructed in an analogous manner, *i.e.*, linking three modulators which bind to three nearby regions on the target to form a multilinked consolidated modulator that has an even higher affinity for the target than the linked modulator. In this example, it
20 is assumed that is desirable to have the modulator bind to all the druggable regions. However, it can be the case that binding to certain of the druggable regions is not desirable, so that the same techniques can be used to identify modulators and consolidated modulators that show increased specificity based on binding to at least one but not all druggable regions of a target.

25 The present invention provides a number of methods that use drug design as described above. For example, in one aspect, the present invention contemplates a method for designing a candidate compound for screening for inhibitors of a polypeptide of the invention, the method comprising: (a) determining the three dimensional structure of a crystallized polypeptide of the invention or a fragment thereof; and (b) designing a
30 candidate inhibitor based on the three dimensional structure of the crystallized polypeptide or fragment.

-98-

In another aspect, the present invention provides a method for identifying a potential inhibitor of a polypeptide of the invention, the method comprising: (a) providing the three-dimensional coordinates of a polypeptide of the invention or a fragment thereof; (b) identifying a druggable region of the polypeptide or fragment; and (c) selecting from a database at least one compound that comprises three dimensional coordinates which indicate that the compound can bind the druggable region; (d) wherein the selected compound is a potential inhibitor of a polypeptide of the invention.

In another aspect, the present invention contemplates a method for identifying a potential modulator of a molecule comprising a druggable region similar to that of SEQ ID NO: 2 or SEQ ID NO: 4, the method comprising: (a) using the atomic coordinates of amino acid residues from SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof, \pm a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5 Å, to generate a three-dimensional structure of a molecule comprising a druggable region that is a portion of SEQ ID NO: 2 or SEQ ID NO: 4; (b) employing the three dimensional structure to design or select the potential modulator; (c) synthesizing the modulator; and (d) contacting the modulator with the molecule to determine the ability of the modulator to interact with the molecule.

In another aspect, the present invention contemplates an apparatus for determining whether a compound is a potential inhibitor of a polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, the apparatus comprising: (a) a memory that comprises: (i) the three dimensional coordinates and identities of the atoms of a polypeptide of the invention or a fragment thereof that form a druggable site; and (ii) executable instructions; and (b) a processor that is capable of executing instructions to: (i) receive three-dimensional structural information for a candidate compound; (ii) determine if the three-dimensional structure of the candidate compound is complementary to the structure of the interior of the druggable site; and (iii) output the results of the determination.

In another aspect, the present invention contemplates a method for designing a potential compound for the prevention or treatment of a disease

-99-

or disorder, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide of the invention, or a fragment thereof; (b) synthesizing a potential compound for the prevention or treatment of a disease or disorder based on the three dimensional structure of the crystallized polypeptide or fragment; (c) contacting a polypeptide of the present invention or a PDE with the potential compound; and (d) assaying the activity of a polypeptide of the present invention, wherein a change in the activity of the polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

In another aspect, the present invention contemplates a method for designing a potential compound for the prevention or treatment of a disease or disorder, the method comprising: (a) providing structural information of a druggable region derived from NMR spectroscopy of a polypeptide of the invention, or a fragment thereof; (b) synthesizing a potential compound for the prevention or treatment of a disease or disorder based on the structural information; (c) contacting a polypeptide of the present invention or a PDE with the potential compound; and (d) assaying the activity of a polypeptide of the present invention, wherein a change in the activity of the polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

X.B. Methods of Designing CAR LBD Ligand Compounds

As discussed above, the analysis of the CAR X-ray structure suggests that CAR can adopt at least two major conformations. One major conformation corresponds to the activated state of CAR, where helix-X is absent, and where the AF2 helix is properly formed and resides in its active position. The second major conformation corresponds to the inactivated conformation, exemplified by the complex of CAR with Compound 1, where helix-X is present and where the AF2 helix is absent. In both conformations, the ligand-binding pocket is capped by the C-terminal tail, residues 340-348. These residues adopt different conformations in the activated and inactivated states of CAR, effectively covering the pocket with a cap that can assume at

-100-

least two alternative shapes. Some CAR ligands might bind preferentially to the activated conformation of CAR, whereas some other CAR ligands might bind preferentially to the inactivated conformation of CAR. There might also be some ligands that bind equally well to either conformation of CAR. When a
5 ligand binds preferentially to a particular conformational state, it will lower the energy of that state, thereby shifting the equilibrium towards that state, and increasing the fraction of the CAR receptor that exists in that state. This thermodynamic principle can be used together with the three dimensional structure of CAR to design chemical compounds that bind to specific
10 conformational states of CAR, thereby increasing or decreasing the level of transcription in genes regulated by CAR.

The present X-ray structure of CAR bound to Compound 1 provides an accurate three-dimensional structure of the ligand-binding pocket in the inactivated conformational state of CAR. Novel ligands can be designed to fit
15 this specific pocket using a variety of computational methods, discussed below. Alternatively, known ligands can be docked into the ligand-binding pocket, using a variety of docking programs and algorithms. These docked structures can be examined graphically to suggest chemical modifications that would improve their fit to the pocket, or their binding to the receptor.
20 Alternatively, known ligands can be complexed with the CAR protein and crystallized using the methods of this invention, allowing the structure of the complex to be determined by X-ray crystallography. The three dimensional structures can be examined graphically to suggest chemical modifications that would improve their fit to the pocket, or their binding to the receptor.

25 The present X-ray structure of CAR can also be used as a template to build a three-dimensional model of the structure of the activated form of CAR. For example, residues 107 to 332, corresponding to helix-1 through most of helix-10, are taken to have exactly the same coordinates as in the template CAR structure. The AF2 helix, CAR residues 341-348, is then built using the
30 structure of VDR as the template. The VDR template structure is superimposed onto the CAR structure using standard methods as disclosed herein and as would be apparent to one of ordinary skill in the art after a

-101-

review of the present disclosure. The AF2 helix from VDR, residues 416-423, is then removed from the VDR template and transplanted into the model for CAR, without any adjustment of its coordinates. Five of the residues in the VDR AF2 helix have amino acid types different from the corresponding
5 residues in the CAR AF2 helix. These residues are VDR Val418, Leu419, Val421, Phe422, and Gly423, which correspond to CAR Leu343, Gln344, Ile346, Cys347, and Ser348, respectively. These five residues are computationally "mutated" in the model, to obtain the covalent structure corresponding to the desired amino acids in CAR. The C-terminal Ser348 is
10 further modified to obtain a free carboxylate as normally occurs at the C-terminal end of a protein chain.

These computational mutations can be carried out using amino acid replacement and builder functionality in molecular graphics programs such as Insight-II, available from Accelrys, or using non-graphical molecular
15 mechanics software such as MVP. The side-chain conformations are then adjusted using computer graphics, such as Insight-II, or other energy-based procedures, such as in MVP, to obtain a reasonable overall fit. It is more difficult to obtain a reasonable conformation for the eight residues in the AF2 linker, CAR residues 333-340. The VDR linker, residues 407-415, cannot be
20 used as the template for the CAR linker because it has nine residues, and because its N-terminal end-point is different from that required in CAR. Likewise, the PXR linker, residues 418-422, is too short to serve as a template for the CAR linker. For structure-based drug design, a conservative approach is to omit the linker residues rather than to model the linker
25 incorrectly. Consequently, in one embodiment the linker, residues 333-340, is omitted from the activated CAR model. This model for the activated state of CAR then provides a binding site for the ligand design processes described elsewhere herein. Specifically, various computer software programs can be used to design novel ligands that would fit the specific pocket in the model for
30 the activated form of CAR. Docking calculations can be used to predict how known CAR activators will bind to the activated form of CAR or to identify other available compounds that might bind. These predicted complex

-102-

structures can then be examined by computer graphics to suggest specific chemical modifications that would enhance the binding to the activated state of CAR.

To be useful as a therapeutic agent, a chemical compound that acts through CAR must induce the appropriate level of CAR activity in relevant tissues. In principle, this can be achieved by adjusting the CAR conformational equilibrium so that appropriate fractions of the CAR protein exist in the activated and inactivated states. This in turn can be achieved with ligands that bind almost exclusively to one or the other of the two major conformational states. The design of ligands that are selective for a specific conformational state is facilitated by consideration of how these ligands might bind to each of the two conformational states. Binding modes can be obtained using docking calculations, and then examined graphically to suggest chemical modifications that would make binding to a particular conformational state either more favorable or less favorable. Iterative application of these techniques can yield ligands with the desired level of selectivity for the particular conformational state of CAR, thereby achieving the desired level of CAR activity. Ligands that can bind to both conformational states of the CAR protein can also be designed. This is also facilitated by consideration of how the ligands might bind to each of the two conformational states, using the same approach as discussed above, but this time seeking chemical structures and chemical modifications that would permit binding to both conformational states.

The methods of this invention can also be used to suggest possible chemical modifications of a compound that might reduce or minimize its effect on CAR. This approach can be useful in drug discovery projects aiming to find compounds that modulate the activity of some other target molecule, where modulation of CAR activity is an undesirable side effect. This approach is useful in engineering CAR activity out of other, non-drug molecules. Humans and other animals are exposed to a wide range of different chemical compounds, some of which might act on CAR in an undesirable manner. Such a compound could be complexed with CAR and crystallized using the

-103-

methods of the present invention. The structure could then be determined by X-ray crystallography. Alternatively, the structure of the complex could be predicted computationally using molecular docking software. In this case, compounds that tend to activate CAR would be docked into a model or structure of the activated form of CAR, whereas compounds that tend to
5 reduce the activity of CAR would be docked into a model or structure of an inactivated form of CAR, such as its complex with Compound 1 presented here.

Whether the structure is obtained by X-ray crystallography or
10 computational methods, the structure would be examined by computer graphics to suggest chemical modifications that would minimize the tendency to bind to CAR. For example, substituents could be introduced onto the compound that would project into volume occupied by the CAR protein. Alternatively, a region of the molecule that binds to a lipophilic region of the
15 CAR binding site could be modified to make it more polar, thus reducing its tendency to bind to CAR. Alternatively, a polar group of the compound that makes a hydrogen bonding interaction with CAR could be identified and modified to an alternative group that fails to make the hydrogen bond. Appropriate chemical modifications can be chosen such that the desirable
20 properties and behavior of the compound would be retained.

The design of candidate substances, also referred to as "compounds" or "candidate compounds", that bind to or modulate nuclear receptor (NR) LBD (for example, CAR LBD) -mediated activity according to the present invention generally involves consideration of two factors. First, the compound
25 must be capable of chemically and structurally associating with a NR LBD. Non-covalent molecular interactions important in the association of a NR LBD with its substrate include hydrogen bonding, van der Waals interactions, and hydrophobic interactions. The interaction between an atom of an LBD amino acid and an atom of an LBD ligand can be made by any force or attraction
30 described in nature. Usually the interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der Waals interaction, or dipole

-104-

interaction. In the case of the hydrophobic interaction, it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic groups from a hydrophobic surface. Reducing or enhancing the interaction of the LBD and a ligand can be measured by calculating or testing binding energies, either computationally or using thermodynamic or kinetic methods known in the art.

Second, the compound must be able to assume a conformation that allows it to associate with a NR LBD. Although certain portions of the compound will not directly participate in this association with a NR LBD, those portions can still influence the overall conformation of the molecule. This influence on conformation, in turn, can have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., the ligand-binding pocket or an accessory binding site of a NR LBD, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with a NR LBD.

Chemical modifications can enhance or reduce interactions of an atom of a LBD amino acid and an atom of an LBD ligand. Steric hindrance can be a common approach for changing the interaction of a LBD binding pocket with an activation domain. Chemical modifications are introduced in one embodiment at C-H, C-, and C-OH positions in a ligand, where the carbon is part of the ligand structure that remains the same after modification is complete. In the case of C-H, C could have 1, 2, or 3 hydrogens, but usually only one hydrogen will be replaced. The H or OH can be removed after modification is complete and replaced with a desired chemical moiety.

The potential binding effect of a chemical compound on a NR LBD can be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques that employ the coordinates of a crystalline NR LBD, for example a CAR LBD polypeptide of the present invention. If the theoretical structure of the given compound suggests insufficient interaction and

-105-

association between it and a NR LBD, synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule can then be synthesized and tested for its ability to bind and modulate the activity of a NR LBD. In this manner, synthesis of unproductive or inactive compounds can be avoided.

A binding compound of a NR LBD polypeptide (in one embodiment a CAR LBD) can be computationally evaluated and designed via a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with an individual binding site or other area of a crystalline CAR LBD polypeptide of the present invention and to interact with the amino acids disposed in the binding sites.

Interacting amino acids forming contacts with a ligand and the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer as discussed herein and in McRee, 1993. However distances can be determined manually once the three dimensional model is made. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. A ligand can also interact with distant amino acids, after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make a new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand. Distant amino acids rarely line the surface of the binding cavity for the ligand, as they are too far away from the ligand to be part of a pocket or surface of the binding cavity.

A compound designed or selected as binding to an NR polypeptide (in one embodiment a CAR LBD polypeptide) can be further computationally optimized so that in its bound state it would lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the ligand and the polypeptide when the ligand is bound

-106-

to an NR LBD make a neutral or favorable contribution to the enthalpy of binding.

One of several methods can be used to screen chemical entities or fragments for their ability to associate with a NR LBD and, more particularly,
5 with the individual binding sites of a NR LBD, such as a ligand-binding pocket or an accessory binding site. This process can begin by visual inspection of, for example, a ligand-binding pocket on a computer screen based on the CAR LBD atomic coordinates disclosed in Tables 2-3. Selected fragments or chemical entities can then be positioned in a variety of orientations, or
10 docked, within an individual binding site of a CAR LBD as defined herein above. Docking can be accomplished using software programs such as those available under the trade names QUANTA™ (available from Accelrys Inc, San Diego, California, United States of America) and SYBYL™ (available from Tripos, Inc., St. Louis, Missouri, United States of America), followed by energy
15 minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARM (Brooks *et al.*, 1993) and AMBER 5 (Case *et al.*, 1997; Pearlman *et al.*, 1995).

Specialized computer programs can also assist in the process of selecting fragments or chemical entities. These include:

- 20 1. GRID™ program, version 17 (Goodford, 1985), which is available from Molecular Discovery Ltd. of Oxford, United Kingdom;
2. MCSS™ program (Miranker & Karplus, 1991), which is available from Accelrys Inc, San Diego, California, United States of America;
3. AUTODOCK™ 3.0 program (Goodsell & Olsen, 1990), which is
25 available from the Scripps Research Institute, La Jolla, California, United States of America;
4. DOCK™ 4.0 program (Kuntz *et al.*, 1992), which is available from the University of California, San Francisco, California, United States of America;
- 30 5. FLEX-X™ program (See Rarey *et al.*, 1996), which is available from Tripos, Inc., St. Louis, Missouri, United States of America;
6. MVP program (Lambert, 1997); and

-107-

7. LUDI™ program (Bohm, 1992), which is available from Accelrys Inc, San Diego, California, United States of America.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or ligand. Assembly can proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a CAR LBD in complex with a co-regulator, optionally in further complex with a ligand. Manual model building using software such as QUANTA™ or SYBYL™ typically follows.

Useful programs to aid one of ordinary skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT™ program (Bartlett *et al.*, 1989), which is available from the University of California, Berkeley, California, United States of America;

2. 3D Database systems, such as MACCS-3D™ system program, which is available from MDL Information Systems, San Leandro, California, United States of America. This area is reviewed in Martin, 1992; and

3. HOOK™ program (Eisen *et al.*, 1994), which is available from Accelrys Inc, San Diego, California, United States of America.

Instead of proceeding to build a NR LBD polypeptide ligand (in one embodiment a CAR LBD ligand) in a step-wise fashion one fragment or chemical entity at a time as described above, ligand compounds can be designed as a whole or *de novo* using the structural coordinates of a crystalline CAR LBD polypeptide of the present invention and either an empty binding site or optionally including some portion(s) of a known ligand(s).

Applicable methods can employ the following software programs:

1. LUDI™ program (Bohm, 1992), which is available from Accelrys Inc, San Diego, California, United States of America;

2. LEGEND™ program (Nishibata & Itai, 1991); and

3. LEAPFROG™, which is available from Tripos Associates, St. Louis, Missouri, United States of America.

Other molecular modeling techniques can also be employed in accordance with this invention. See *e.g.*, Cohen *et al.*, 1990; Navia & Murcko,

-108-

1992; and U.S. Patent No. 6,008,033 to Abdel-Meguid et al., all of which are incorporated herein by reference.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound can bind to a NR LBD can be tested and optimized by computational evaluation. By way of a particular example, a compound that has been designed or selected to function as a CAR LBD ligand can traverse a volume not overlapping that occupied by the binding site when it is bound to its native ligand. Additionally, an effective NR LBD ligand can demonstrate a relatively small difference in energy between its bound and free states (*i.e.*, a small deformation energy of binding). Thus, the most efficient NR LBD ligands can be designed with a deformation energy of binding of in one embodiment not greater than about 10 kcal/mole, and in another embodiment not greater than 7 kcal/mole. It is possible for NR LBD ligands to interact with the polypeptide in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the thermodynamic average energy of the conformations observed when the ligand binds to the polypeptide.

A compound designed or selected as binding to a NR LBD polypeptide (preferably a CAR polypeptide, more preferably a CAR LBD polypeptide) can be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (*e.g.*, electrostatic) interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the ligand and the polypeptide when the ligand is bound to a NR LBD preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include:

1. GAUSSIAN 98™, which is available from Gaussian, Inc., Pittsburgh, Pennsylvania, United States of America;

-109-

2. AMBER™ program, version 6.0, which is available from the University of California, San Francisco, California, United States of America;

3. QUANTA™ program, which is available from Accelrys Inc, San Diego, California, United States of America;

5 4. CHARMM® program, which is available from Accelrys Inc, San Diego, California, United States of America; and

4. INSIGHT II® program, which is available from Accelrys Inc, San Diego, California, United States of America.

10 These programs can be implemented using a suitable computer system. Other hardware systems and software packages will be apparent to those skilled in the art after review of the disclosure of the present invention presented herein.

15 Once a NR LBD modulating compound has been optimally selected or designed, as described above, substitutions can then be made in some of its atoms or side groups in order to improve or modify its binding properties. In some cases, initial substitutions might be conservative, e.g., the replacement group will have approximately the same size, shape, hydrophobicity, and charge as the original group. In other cases, the replacement group will have different properties as desired to make specific interactions with the protein.

20 Such substituted chemical compounds can then be analyzed for efficiency of fit to a NR LBD binding site using the same computer-based approaches described in detail above.

X.C. Sterically Similar Compounds

25 A further aspect of the present invention is that sterically similar compounds can be formulated to mimic the key portions of a CAR LBD structure. Such compounds are functional equivalents. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described

30 herein. Modeling and chemical design of CAR and CAR LBD structural equivalents can be based on the structure coordinates of a crystalline CAR

-110-

LBD polypeptide of the present invention. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

XI. CAR Polypeptides

5 The generation of mutant and chimeric CAR polypeptides is also an aspect of the present invention. A chimeric polypeptide can comprise a CAR LBD polypeptide or a portion of a CAR LBD, (e.g. a CAR LBD) which is fused to a candidate polypeptide or a suitable region of the candidate polypeptide. Throughout the present disclosure it is intended that the term "mutant"

10 encompass not only mutants of a CAR LBD polypeptide but chimeric proteins generated using a CAR LBD as well. It is thus intended that the following discussion of mutant CAR LBDs apply *mutatis mutandis* to chimeric CAR and CAR LBD polypeptides and to structural equivalents thereof.

 In accordance with the present invention, a mutation can be directed to

15 a particular site or combination of sites of a wild-type CAR LBD. For example, an accessory binding site or the binding pocket can be chosen for mutagenesis. Similarly, a residue having a location on, at or near the surface of the polypeptide can be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type CAR and CAR LBD.

20 Alternatively, an amino acid residue in a CAR or a CAR LBD can be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

 Such mutants can be characterized by any one of several different properties as compared with the wild-type CAR LBD. For example, such mutants can have an altered surface charge of one or more charge units, or

25 can have an increase in overall stability. Other mutants can have altered ligand specificity in comparison with, or a higher specific activity than, a wild type CAR or CAR LBD.

 CAR and CAR LBD mutants of the present invention can be generated in a number of ways. For example, the wild-type sequence of a CAR or a

30 CAR LBD can be mutated at those sites identified using this invention as desirable for mutation by employing oligonucleotide-directed mutagenesis or other conventional methods. Alternatively, mutants of a CAR or a CAR LBD

-111-

can be generated by the site-specific replacement of a particular amino acid with an unnaturally occurring amino acid. In addition, CAR or CAR LBD mutants can be generated through replacement of an amino acid residue, for example, a particular cysteine or methionine residue, with selenocysteine or selenomethionine. This can be achieved by growing a host organism capable of expressing either the wild type or mutant polypeptide on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

Mutations can be introduced into a DNA sequence coding for a CAR or a CAR LBD using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites. Mutations can be generated in the full-length DNA sequence of a CAR or a CAR LBD or in any sequence coding for polypeptide fragments of a CAR or a CAR LBD.

According to the present invention, a mutated CAR or CAR LBD DNA sequence produced by the methods described above, or any alternative methods known in the art, can be expressed using an expression vector. An expression vector, as is well known to those of skill in the art, typically includes elements that permit autonomous replication in a host cell independent of the host genome, and one or more phenotypic markers for selection purposes. Either prior to or after insertion of the DNA sequences surrounding the desired CAR or CAR LBD mutant coding sequence, an expression vector includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes and a signal for termination. Where secretion of the produced mutant is desired, nucleotides encoding a "signal sequence" can be inserted prior to a CAR or a CAR LBD mutant coding sequence. For expression under the direction of the control sequences, a desired DNA sequence is operatively linked to the control sequences; that is, the sequence has an appropriate start signal in front of the DNA sequence encoding the CAR or CAR LBD mutant, and the correct reading frame to permit expression of that sequence under the control of the control sequences and production of the desired product encoded by that CAR or CAR LBD sequence.

-112-

Any of a wide variety of well-known available expression vectors can be used to express a mutated CAR or CAR LBD coding sequences of this invention. These include for example, vectors consisting of segments of chromosomal, non-chromosomal, and synthetic DNA sequences, such as known derivatives of SV40, known bacterial plasmids, *e.g.*, plasmids from *E. coli* including colE1, pCR1, pBR322, pMB9 and their derivatives, wider host range plasmids, *e.g.*, RP4, phage DNAs, *e.g.*, derivatives of phage λ , *e.g.*, NM 989, and other DNA phages, *e.g.*, M13 and filamentous single stranded DNA phages, yeast plasmids and vectors derived from combinations of plasmids and phage DNAs, such as plasmids which have been modified to employ phage DNA or other expression control sequences. In one embodiment of the present invention, a vector amenable to expression in a pRSETA-based expression system is employed. The pRSETA expression system is available from Invitrogen, Inc., Carlsbad, California, United States of America.

In addition, any of a wide variety of expression control sequences – *i.e.* sequences that control the expression of a DNA sequence when operatively linked to it – can be used in these vectors to express the mutated DNA sequences according to this invention. Such useful expression control sequences, include, but are not limited to the early and late promoters of SV40 for animal cells; the lac system, the trp system, the TAC or TRC system, the major operator and promoter regions of phage λ , and the control regions of fd coat protein for *E. coli*; the promoter for 3-phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, (for example, Pho5), and the promoters of the yeast α -mating factors for yeast; as well as other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof.

A wide variety of hosts can be employed for producing mutated CAR and CAR LBD polypeptides according to this invention. These hosts include, for example, bacteria, such as *E. coli*, *Bacillus*, and *Streptomyces*; fungi, such

-113-

as yeasts; animal cells, such as CHO and COS-1 cells; plant cells; insect cells, such as Sf9 cells; and transgenic host cells.

It should be understood that not all expression vectors and expression systems function in the same way to express mutated DNA sequences of this invention, and to produce modified CAR and CAR LBD polypeptides or CAR or CAR LBD mutants. Neither do all hosts function equally well with the same expression system. One of skill in the art can, however, make a selection among these vectors, expression control sequences and hosts without undue experimentation and without departing from the scope of this invention. For example, an important consideration in selecting a vector will be the ability of the vector to replicate in a given host. The copy number of the vector, the ability to control that copy number, and the expression of any other proteins encoded by the vector, such as antibiotic markers, should also be considered.

In selecting an expression control sequence, a variety of factors should also be considered. These include, for example, the relative strength of the system, its controllability and its compatibility with the DNA sequence encoding a modified CAR or CAR LBD polypeptide of this invention, with particular regard to the formation of potential secondary and tertiary structures.

Hosts should be selected by consideration of their compatibility with the chosen vector, the toxicity of a modified CAR or CAR LBD to them, their ability to express mature products, their ability to fold proteins correctly, their fermentation requirements, the ease of purification of a modified CAR or CAR LBD and safety. Within these parameters, one of skill in the art can select various vector/expression control system/host combinations that will produce useful amounts of a mutant CAR or CAR LBD. A mutant CAR or CAR LBD produced in these systems can be purified by a variety of conventional steps and strategies, including those used to purify the wild type CAR or CAR LBD.

Once a CAR LBD mutation(s) has been generated in the desired location, such as an active site or dimerization site, the mutants can be tested for any one of several properties of interest. For example, mutants can be screened for an altered charge at physiological pH. This is determined by

-114-

measuring the mutant CAR or CAR LBD isoelectric point (pI) and comparing the observed value with that of the wild-type parent. Isoelectric point can be measured by gel-electrophoresis according to the method of Wellner, 1971. A mutant CAR or CAR LBD polypeptide containing a replacement amino acid
5 located at the surface of the enzyme, as provided by the structural information of this invention, can lead to an altered surface charge and an altered pI.

XI.A. Generation of an Engineered CAR LBD or CAR LBD Mutant

In an embodiment of the present invention, a unique CAR or CAR LBD
10 polypeptide is generated. Such a mutant can facilitate purification and the study of the ligand-binding abilities of a CAR polypeptide.

As used in the following discussion, the terms "engineered CAR", "engineered CAR LBD", "CAR mutant", and "CAR LBD mutant" refers to polypeptides having amino acid sequences which contain at least one
15 mutation in the wild-type sequence. The terms also refer to CAR and CAR LBD polypeptides which are capable of exerting a biological effect in that they comprise all or a part of the amino acid sequence of an engineered CAR or CAR LBD polypeptide of the present invention, or cross-react with antibodies raised against an engineered CAR or CAR LBD polypeptide, or retain all or
20 some or an enhanced degree of the biological activity of the engineered CAR or CAR LBD amino acid sequence or protein. Such biological activity can include the binding of small molecules in general, and the binding of Compound 1, in particular.

The terms "engineered CAR LBD" and "CAR LBD mutant" also
25 includes analogs of an engineered CAR LBD or CAR LBD polypeptide. By "analog" is intended that a DNA or polypeptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some or an enhanced degree of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences or from other organisms,
30 or can be created synthetically. Those of skill in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct CAR LBD or CAR LBD mutant analogs. There is no need for

-115-

a CAR LBD or CAR LBD mutant polypeptide to comprise all or substantially all of the amino acid sequence of SEQ ID NOs: 2 or 4. Shorter or longer sequences can be employed in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "engineered CAR LBD" and "CAR LBD mutant" also includes fusion, chimeric or recombinant CAR LBD or CAR LBD mutant polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein above and are known in the art.

10 XI.A.1. Sequences That Are Substantially Identical to a CAR or
CAR LBD Mutant Sequence of the Present Invention

Nucleic acids that are substantially identical to a nucleic acid sequence of a CAR or CAR LBD mutant of the present invention, *e.g.* allelic variants, genetically altered versions of the gene, etc., bind to a CAR or CAR LBD mutant sequence under stringent hybridization conditions. By using probes, particularly labeled probes of DNA sequences, one can isolate homologous or related genes. The source of homologous genes can be any organism, including, but not limited to primates; rodents, such as rats and mice; canines; felines; bovines; equines; yeast; and nematodes.

20 Among mammalian species, *e.g.* human and mouse, homologs can
have substantial sequence similarity, *i.e.* at least 75% sequence identity
between nucleotide sequences. Sequence similarity is calculated based on a
reference sequence, which can be a subset of a larger sequence, such as a
conserved motif, coding region, flanking region, etc. In one embodiment, a
25 reference sequence is at least about 18 nucleotides (nt) long, in another
embodiment at least about 30 nt long, and can extend to the complete
sequence that is being compared. Algorithms for sequence analysis are
known in the art, such as BLAST, described in Altschul *et al.*, 1990.

Percent identity or percent similarity of a DNA or peptide sequence can
30 be determined, for example, by comparing sequence information using the
GAP computer program, available from the University of Wisconsin Genetics
Computer Group (now part of Accelrys Inc, San Diego, California, United

-116-

States of America). The GAP program utilizes the alignment method of Needleman *et al.*, 1970, as revised by Smith *et al.*, 1981. Briefly, the GAP program defines similarity as the number of aligned symbols (*i.e.*, nucleotides or amino acids) that are similar, divided by the total number of symbols in the shorter of the two sequences. The preferred parameters for the GAP program are the default parameters, which do not impose a penalty for end gaps. See *e.g.*, Schwartz *et al.*, 1979; Gribskov *et al.*, 1986.

The term "similarity" is contrasted with the term "identity". Similarity is defined as above; "identity", however, refers to a nucleic acid or amino acid sequence having the same amino acid at the same relative position in a given family member of a gene family. Homology and similarity are generally viewed as broader terms than the term identity. Biochemically similar amino acids, for example leucine/isoleucine or glutamate/aspartate, can be present at the same position – these are not identical per se, but are biochemically "similar." As disclosed herein, these are referred to as conservative differences or conservative substitutions. This differs from a conservative mutation at the DNA level, which changes the nucleotide sequence without making a change in the encoded amino acid, *e.g.* TCC to TCA, both of which encode serine.

As used herein, DNA analog sequences are "substantially identical" to specific DNA sequences disclosed herein if: (a) the DNA analog sequence is derived from coding regions of the nucleic acid sequence shown in SEQ ID NOs: 1 or 3; or (b) the DNA analog sequence is capable of hybridization with DNA sequences of (a) under stringent conditions and which encode a biologically active CAR or CAR LBD gene product; or (c) the DNA sequences are degenerate as a result of alternative genetic code to the DNA analog sequences defined in (a) and/or (b). Substantially identical analog proteins and nucleic acids will have between about 70% and 80%, preferably between about 81% to about 90% or even more preferably between about 91% and 99% sequence identity with the corresponding sequence of the native protein or nucleic acid. Sequences having lesser degrees of identity but comparable biological activity are considered to be equivalents.

-117-

As used herein, "stringent conditions" refers to conditions of high stringency, for example 6X SSC, 0.2% polyvinylpyrrolidone, 0.2% Ficoll, 0.2% bovine serum albumin, 0.1% sodium dodecyl sulfate, 100 µg/ml salmon sperm DNA and 15% formamide at 68°C. For the purposes of specifying additional
5 conditions of high stringency, preferred conditions comprise a salt concentration of about 200 mM and temperature of about 45°C. One example of stringent conditions is hybridization in 4X SSC, at 65°C, followed by a washing in 0.1X SSC at 65°C for one hour. Another exemplary stringent hybridization scheme uses 50% formamide, 4X SSC at 42°C.

10 In contrast, nucleic acids having sequence similarity are detected by hybridization under lower stringency conditions. Thus, sequence identity can be determined by hybridization under lower stringency conditions, for example, at 50°C or higher and 0.1X SSC (9 mM NaCl/0.9 mM sodium citrate) and the sequences will remain bound when subjected to washing at 55°C in
15 1X SSC.

XI.A.2. Complementarity and Hybridization to an Engineered
CAR or CAR LBD Mutant Sequence

As used herein, the term "functionally equivalent codon" is used to refer
20 to codons that encode the same amino acid, such as the ACG and AGU codons for serine. CAR or CAR LBD-encoding nucleic acid sequences comprising SEQ ID NOs: 1 and 3, which have functionally equivalent codons are covered by the present invention. Thus, when referring to the sequence examples presented in SEQ ID NOs: 1 and 3, applicants contemplate
25 substitution of functionally equivalent codons into the sequence example of SEQ ID NOs: 1 and 3. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

It will also be understood by those of skill in the art that amino acid and
30 nucleic acid sequences can include additional residues, such as additional N- or C-terminal amino acids or 5' or 3' nucleic acid sequences, and yet still be essentially as set forth in one of the sequences disclosed herein, so long as

-118-

the sequence retains biological protein activity where polypeptide expression is concerned. The addition of terminal sequences particularly applies to nucleic acid sequences which can, for example, include various non-coding sequences flanking either of the 5' or 3' portions of the coding region or can
5 include various internal sequences, *i.e.*, introns, which are known to occur within genes.

XI.B. Biological Equivalents

The present invention envisions and includes biological equivalents of
10 CAR or CAR LBD mutant polypeptide of the present invention. The term "biological equivalent" refers to proteins having amino acid sequences which are substantially identical to the amino acid sequence of a CAR LBD mutant of the present invention and which are capable of exerting a biological effect in that they are capable of binding a small molecule, binding a co-regulator,
15 homo- or heterodimerizing or cross-reacting with anti-CAR or CAR LBD mutant antibodies raised against a mutant CAR or CAR LBD polypeptide of the present invention.

For example, certain amino acids can be substituted for other amino acids in a protein structure without appreciable loss of interactive capacity
20 with, for example, structures in the nucleus of a cell. Since it is the interactive capacity and nature of a protein that defines that protein's biological functional activity, certain amino acid sequence substitutions can be made in a protein sequence (or the nucleic acid sequence encoding it) to obtain a protein with the same, enhanced, or antagonistic properties. Such properties can be
25 achieved by interaction with the normal targets of the protein, but this need not be the case, and the biological activity of the invention is not limited to a particular mechanism of action. It is thus in accordance with the present invention that various changes can be made in the amino acid sequence of a CAR or CAR LBD mutant polypeptide of the present invention or its
30 underlying nucleic acid sequence without appreciable loss of biological utility or activity.

-119-

Biologically equivalent polypeptides, as used herein, are polypeptides in which certain, but not most or all, of the amino acids can be substituted. Thus, when referring to the sequence examples presented in SEQ ID NOs: 2 and 4, applicants envision substitution of codons that encode biologically
5 equivalent amino acids, as described herein, into the sequence example of SEQ ID NOs: 2 and 4, respectively. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

Alternatively, functionally equivalent proteins or peptides can be
10 created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged, e.g. substitution of Ile for Leu. Changes designed by man can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the
15 antigenicity of the protein or to test a CAR or CAR LBD mutant polypeptide of the present invention in order to modulate co-regulator-binding or other activity, at the molecular level.

Amino acid substitutions, such as those which might be employed in modifying a CAR or CAR LBD mutant polypeptide of the present invention are
20 generally, but not necessarily, based on the relative similarity of the amino acid side-chain substituents, for example, their hydrophobicity, hydrophilicity, charge, size, and the like. An analysis of the size, shape and type of the amino acid side-chain substituents reveals that arginine, lysine and histidine are all positively charged residues; that alanine, glycine and serine are all of
25 similar size; and that phenylalanine, tryptophan and tyrosine all have a generally similar shape. Therefore, based upon these considerations, arginine, lysine and histidine; alanine, glycine and serine; and phenylalanine, tryptophan and tyrosine; are defined herein as biologically functional equivalents. Those of skill in the art will appreciate other biologically
30 functional equivalent changes. It is implicit in the above discussion, however, that one of skill in the art can appreciate that a radical, rather than a conservative substitution is warranted in a given situation. Non-conservative

-120-

substitutions in mutant CAR or CAR LBD polypeptides of the present invention are also an aspect of the present invention.

In making biologically functional equivalent amino acid substitutions, the hydrophobic index of amino acids can be considered. Each amino acid
5 has been assigned a hydrophobic index on the basis of their hydrophobicity and charge characteristics, these are: isoleucine (+ 4.5); valine (+ 4.2); leucine (+ 3.8); phenylalanine (+ 2.8); cysteine (+ 2.5); methionine (+ 1.9); alanine (+ 1.8); glycine (-0.4); threonine (-0.7); serine (-0.8); tryptophan (-0.9); tyrosine (-1.3); proline (-1.6); histidine (-3.2); glutamate (-3.5); glutamine (-
10 3.5); aspartate (-3.5); asparagine (-3.5); lysine (-3.9); and arginine (-4.5).

The importance of the hydrophobic amino acid index in conferring interactive biological function on a protein is generally understood in the art (Kyte & Doolittle, 1982, incorporated herein by reference). It is known that certain amino acids can be substituted for other amino acids having a similar
15 hydrophobic index or score and still retain a similar biological activity. In making changes based upon the hydrophobic index, the substitution of amino acids whose hydrophobic indices are within ± 2 of the original value is preferred, those within ± 1 of the original value are particularly preferred, and those within ± 0.5 of the original value are even more particularly preferred.

It is also understood in the art that the substitution of like amino acids
20 can be made effectively on the basis of hydrophilicity. U.S. Patent No. 4,554,101, incorporated herein by reference, states that the greatest local average hydrophilicity of a protein, as governed by the hydrophilicity of its adjacent amino acids, correlates with its immunogenicity and antigenicity, *i.e.*
25 with a biological property of the protein. It is understood that an amino acid can be substituted for another having a similar hydrophilicity value and still obtain a biologically equivalent protein.

As detailed in U.S. Patent No. 4,554,101 to Hopp, the following hydrophilicity values have been assigned to amino acid residues: arginine (+
30 3.0); lysine (+ 3.0); aspartate (+ 3.0 \pm 1); glutamate (+ 3.0 \pm 1); serine (+ 0.3); asparagine (+ 0.2); glutamine (+ 0.2); glycine (0); threonine (-0.4); proline (-0.5 \pm 1); alanine (-0.5); histidine (-0.5); cysteine (-1.0); methionine (-1.3); valine

-121-

(-1.5); leucine (-1.8); isoleucine (-1.8); tyrosine (-2.3); phenylalanine (-2.5); tryptophan (-3.4).

In making changes based upon similar hydrophilicity values, the substitution of amino acids whose hydrophilicity values are within ± 2 of the original value is preferred, those that are within ± 1 of the original value are particularly preferred, and those within ± 0.5 of the original value are even more particularly preferred.

While discussion has focused on functionally equivalent polypeptides arising from amino acid changes, it will be appreciated that these changes can be effected by alteration of the encoding DNA, taking into consideration also that the genetic code is degenerate and that two or more codons can code for the same amino acid.

Thus, it will also be understood that this invention is not limited to the particular amino acid and nucleic acid sequences of SEQ ID NOs: 1-4. Recombinant vectors and isolated DNA segments can therefore variously include a CAR or CAR LBD mutant polypeptide-encoding region itself, include coding regions bearing selected alterations or modifications in the basic coding region, or include larger polypeptides which nevertheless comprise a CAR or CAR LBD mutant polypeptide-encoding regions or can encode biologically functional equivalent proteins or polypeptides which have variant amino acid sequences. Biological activity of a CAR or CAR LBD mutant polypeptide can be determined, for example, by employing binding assays known to those of skill in the art.

The nucleic acid segments of the present invention, regardless of the length of the coding sequence itself, can be combined with other DNA sequences, such as promoters, enhancers, polyadenylation signals, additional restriction enzyme sites, multiple cloning sites, other coding segments, polyhistidine encoding segments and the like, such that their overall length can vary considerably. It is therefore contemplated that a nucleic acid fragment of almost any length can be employed, with the total length preferably being limited by the ease of preparation and use in the intended recombinant DNA protocol. For example, nucleic acid fragments can be

-122-

prepared which include a short stretch complementary to a nucleic acid sequence set forth in SEQ ID NOs: 1 and 3, such as about 10 nucleotides, and which are up to 10,000 or 5,000 base pairs in length. DNA segments with total lengths of about 4,000, 3,000, 2,000, 1,000, 500, 200, 100, and about 50
5 base pairs in length are also useful.

The DNA segments of the present invention encompass biologically functional equivalents of CAR or CAR LBD mutant polypeptides. Such sequences can arise as a consequence of codon redundancy and functional equivalency that are known to occur naturally within nucleic acid sequences and the proteins thus encoded. Alternatively, functionally equivalent proteins
10 or polypeptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged. Changes can be introduced through the application of site-directed mutagenesis techniques, *e.g.*, to introduce improvements to the
15 antigenicity of the protein or to test variants of a CAR or CAR LBD mutant of the present invention in order to examine the degree of lipid-binding activity, or other activity at the molecular level. Various site-directed mutagenesis techniques are known to those of skill in the art and can be employed in the
20 present invention.

The invention further encompasses fusion proteins and peptides wherein a CAR or CAR LBD mutant coding region of the present invention is aligned within the same expression unit with other proteins or peptides having desired functions, such as for purification or immunodetection purposes.

25 Recombinant vectors form important further aspects of the present invention. Particularly useful vectors are those in which the coding portion of the DNA segment is positioned under the control of a promoter. The promoter can be that naturally associated with a CAR gene, as can be obtained by isolating the 5' non-coding sequences located upstream of the coding
30 segment or exon, for example, using recombinant cloning and/or PCR technology and/or other methods known in the art, in conjunction with the compositions disclosed herein.

-123-

In other embodiments, certain advantages can be gained by positioning the coding DNA segment under the control of a recombinant, or heterologous, promoter. As used herein, a recombinant or heterologous promoter is a promoter that is not normally associated with a CAR gene in its natural environment. Such promoters can include promoters isolated from bacterial, viral, eukaryotic, or mammalian cells. Naturally, it will be important to employ a promoter that effectively directs the expression of the DNA segment in the cell type chosen for expression. The use of promoter and cell type combinations for protein expression is generally known to those of skill in the art of molecular biology (See e.g., Sambrook & Russell, 2001, specifically incorporated herein by reference). The promoters employed can be constitutive or inducible and can be used under the appropriate conditions to direct high level expression of the introduced DNA segment, such as is advantageous in the large-scale production of recombinant proteins or peptides. One exemplary promoter system contemplated for use in high-level expression is a T7 promoter-based system.

XII. The Role of the Three-Dimensional Structure of the CAR LDB in Solving Additional CAR Crystals

Because polypeptides can crystallize in more than one crystal form, the structural coordinates of a CAR LBD, or portions thereof, in complex with a co-regulator as provided by the present invention, are particularly useful in solving the structure of other crystal forms of CAR and the crystalline forms of other NRs and CARs. The coordinates provided in the present invention can also be used to solve the structure of CAR or CAR LBD mutants (such as those above), CAR LDB co-complexes, or the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of CAR.

One method that can be employed for the purpose of solving additional CAR crystal structures is molecular replacement. See generally, Rossmann, 1972. In the molecular replacement method, an unknown crystal form, whether it is another crystal form of a CAR or a CAR LBD, (i.e. a CAR or a

-124-

CAR LBD mutant), a CAR or a CAR LBD polypeptide in complex with another compound (*i.e.* a "co-complex") or the crystal of some other protein with significant amino acid sequence homology to any functional region of the CAR LBD (*e.g.* another NR), can be determined using the CAR LBD structure
5 coordinates provided in Tables 2-3. This method provides an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

In addition, in accordance with this invention, CAR or CAR LBD mutants can be crystallized in complex with known modulators, such as a co-
10 regulator. The crystal structures of a series of such complexes can then be solved by molecular replacement and compared with that of wild-type CAR or the wild-type CAR LBD. Potential sites for modification within the various binding sites of the enzyme can thus be conveniently identified. This information provides an additional tool for identifying efficient binding
15 interactions, for example, increased hydrophobic interactions between the CAR LBD and a chemical entity or compound.

All of the complexes referred to in the present disclosure can be studied using X-ray diffraction techniques (See *e.g.*, Blundell & Johnson, 1985) and can be refined using computer software, such as the X-PLOR™
20 program (Brünger, 1992; X-PLOR is available from Accelrys Inc, San Diego, California, United States of America). This information can thus be used to optimize known classes of CAR and CAR LBD ligands, and more importantly, to design and synthesize novel classes of CAR and CAR LBD ligands, including co-regulators.

25

Examples

The following Examples have been included to illustrate exemplary modes of the invention. Certain aspects of the following Examples are described in terms of techniques and procedures found or contemplated by
30 the present inventors to work well in the practice of the invention. These Examples are exemplified through the use of standard laboratory practices of the inventors. In light of the present disclosure and the general level of skill in

-125-

the art, those of skill will appreciate that the following Examples are intended to be exemplary only and that numerous changes, modifications, and alterations can be employed without departing from the spirit and scope of the invention.

5

Example 1

Protein Expression and Purification

A DNA fragment encoding residues 103 - 348 of a human CAR polypeptide (GenBank Accession No. Z30425) was amplified by the
10 polymerase chain reaction (PCR) with a commercial kit (Stratagene, La Jolla, California, United States of America). The 5' PCR primer included an N-terminal poly-histidine tag sequence (MKKGHHHHHG; SEQ ID NO: 5) along with an NdeI endonuclease restriction site (CATATG), and the 3' PCR primer contained a BamHI restriction site (GGATCC). The PCR primers used were
15 5'-CGGCGGCGCCATATGAAAAAGGTCATCATCATCATCATGGTCCT
GTGAACTGAGTAAGGAGCAAG-3' (SEQ ID NO: 6) and 5'-
CGGCGGCGCGGATCCTTAGCTGCAGATCTCCTGGAGCAGCGG 3' (SEQ
ID NO: 7). The amplified DNA fragment was inserted downstream of a T7
promoter from the pRSETA vector (Invitrogen Corp., Carlsbad, California,
20 United States of America) at the NdeI-BamHI enzyme restriction sites. *E. coli* cells BL21(DE3) transformed with the above expression vector were grown on a carbenicillin antibiotic agar plate (50 mg/L carbenicillin). A starter culture of 80 ml LB media (10 g/L Bacto-Tryptone, 5 g/L yeast extract, 5 g/L NaCl, QC with distilled water) with carbenicillin antibiotic (50 mg/L carbenicillin) was
25 grown from one colony at 37°C, 250 rpm for four hours. Twelve 2 L shaker flasks with 1L LB media and carbenicillin antibiotic (50 mg/L carbenicillin) were inoculated with 5 ml of the starter culture. Cells were grown at 23°C, 250 rpm for 16 hours to an OD₆₀₀ of 2.0, and harvested by centrifugation. The pellet was completely resuspended with 20 ml extract buffer (150 mM NaCl,
30 50 mM imidazole pH 7.5) per liter of cells. The cells were sonicated for 5 minutes using a Sonicator Ultrasonic Processor XL-2015 (Heat Systems, Inc., Farmingdale, New York, United States of America) at 0°C. The lysed cells

-126-

were centrifuged at 40,000g for 40 minutes and the supernatant was loaded on a 50 ml Ni-agarose column. The column was washed with 250 ml Buffer A (50 mM imidazole pH 7.5, 150 mM NaCl), 100 ml of Buffer B (200 mM imidazole pH 7.5, 150 mM NaCl), and the protein eluted with a 300 ml gradient to Buffer B (500 mM imidazole pH 7.5, 150 mM NaCl). The peak, which eluted at 45% Buffer B, contained 60 mg of His-tagged CAR LBD protein.

This protein was diluted 5-fold in 10 mM Tris-Cl pH 8.0 to reduce the NaCl concentration before loading the entire sample on a 50 ml SP Sepharose FASTFLOW™ column (Pharmacia Biotech, now part of Amersham Biosciences Corp., Piscataway, New Jersey, United States of America). The column was washed with 200 ml Buffer S-A (10 mM Tris-Cl pH 8.0, 30 mM NaCl, 5 mM DTT, 1 mM EDTA pH 8.0) and the His-tagged CAR protein was eluted from the column by running a 300 ml increasing NaCl concentration gradient of Buffer S-B (10 mM Tris-Cl pH 8.0, 500 mM NaCl, 5 mM DTT, 1 mM EDTA pH 8.0). Peak fractions containing the CAR protein were pooled together, protein was concentrated to 1 mg/ml in CENTRIPREP™ 30 units (Millipore Corp., Bedford, Massachusetts, United States of America) concentrators. The protein yield was 4 mg/L cells grown. The protein was aliquoted into 10 mg aliquots at 1.0 mg/ml and stored on ice.

The purified CAR LBD protein (10 mg) was complexed with Compound 1 (10 mM in DMSO) in a 1:5 molar ratio and incubated on ice for 1 hour. The CAR LBD/Compound 1 protein complex was concentrated to 4 mg/ml in a CENTRIPREP™ 30 units and stored on ice until needed for crystallization efforts.

Example 2

Crystallization and Data Collection

CAR/Compound 1 crystals were grown at 4°C in hanging drops containing 1 µl of the protein-ligand solutions disclosed in Example 1, and 1 µl of well buffer (100 - 400 mM sodium potassium tartrate, pH 7.1 - 7.4). Crystals grew to a size of 100-200 µm within several weeks. Before data

-127-

collection, crystals were transiently mixed with the well buffer that contains an additional 14% ethylene glycol, 7% glycerol, and then flash frozen in liquid nitrogen.

Orthorhombic CAR/ligand crystals formed in the $P2_12_12_1$ space group,
5 with $a=82.3 \text{ \AA}$, $b = 116.8 \text{ \AA}$, $c = 131.9 \text{ \AA}$. Each asymmetric unit contained four CAR LBDs and four ligands. The crystals had a solvent content of 40%.

Crystals were screened with a Rigaku R-Axis IV detector (Rigaku International Corp., Tokyo, Japan), and data sets were collected with a MAR CCD detector at the IMCA 17ID beam line at Argonne National Labs
10 (Argonne, Illinois, United States of America). The observed reflections were reduced, merged, and scaled with DENZOTM and SCALEPACKTM software in the HKL2000 package (Otwinowski, 1993).

Example 3

15 Structure Determination and Refinement

Structures were determined by molecular replacement methods with the CCP4 AMORETM program (Collaborative Computational Project, 1994; Navaza, 1994) using the poly-alanine model of the conserved region of VDR LBD. Coordinates for this model are presented in Table 3.

20 The best fitting solution generated with the AMORETM program gave a correlation coefficient of 30% and an R-factor of 50%. The phases generated from molecular replacement were extensively refined and improved with solvent flattening, histogram matching, and NCS as implemented in CCP4DM and DMMULTI programs (Cowtan, 1994). Model building
25 proceeded with QUANTATM (available from Accelrys Inc, San Diego, California, United States of America), and refinement progressed with CNX (Brünger *et al.*, 1998), and involved multiple cycles of manual rebuilding.

The structure of CAR in complex with the antagonist Compound 1 was determined. The statistics of the structure are summarized in Table 1.

-128-

Example 4

Computational Analysis

Surface area was calculated with the Connolly MS program (Connolly, 1983) and the MVP program (Lambert, 1997). The binding pocket volumes
5 were calculated with the program GRASP (Nicholls *et al.*, 1991), using the program MVP to close openings to solvent. The sequence alignments were generated with the MVP program.

Example 5

Antagonist Assays

10 Screening of synthetic compound libraries with the purified CAR LBD protein by a Fluorescence Resonance Energy Transfer (FRET) Ligand Sensing Assay (Parks *et al.*, 1999) was conducted to identify molecules that alter the basal interaction between a coactivator peptide and the CAR LBD
15 protein. Briefly, the purified human CAR LBD protein was biotinylated and labeled with streptavidin-conjugated fluorophore allophycocyanin. The labeled CAR LBD protein was incubated with a test compound and with a peptide that included the second LXXLL binding motif of the nuclear coactivator SRC-1 (GenBank Accession No. U59302; amino acids 676-700)
20 that was labeled with europium chelate. Data were collected with a WALLAC VICTOR™ fluorescence reader (available from PerkinElmer Life Sciences Inc., Boston, Massachusetts, United States of America) in a time resolved mode and the fluorescence ratio calculated. Compound 1 was identified from the screen to be an inverse agonist molecule that reduces the basal
25 fluorescent signal indicating that the CAR LBD/SRC-1 interaction was reduced below background levels. Standard dose response curves were conducted with the CAR LBD protein plus Compound 1 and the EC₅₀ was determined to be 15 nM.

-129-

Example 6Synthesis of Compound 1

2-(benzhydrylamino) - 1 - (2-phenylethyl) - 1*H* - benzimidazole-6-carboxamide (Compound 1) was synthesized as follows. A solution of 3-fluoro-4-nitrobenzoic acid (1.28 g; 6.9 mmol) in 10 mL anhydrous *N,N*-dimethylformamide was treated with [O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluoro-phosphate] (2.6 g; 6.9 mmol) followed by *N,N*-diisopropylethylamine (3.6 ml, 20.7 mmol). After shaking for 5 min, the mixture was added to polystyrene Rink amide AM resin (1.0 g; 0.69 mmol/g; 0.69 mmol), and the reaction was rotated at 25°C for 18 h. The reaction solution was drained, and the resin was washed sequentially with *N,N*-dimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The dried resin was treated with 15.2 ml of a 0.5 M phenethylamine in *N*-methylpyrrolidinone solution then rotated at 70°C for 15 hours. The cooled reaction was drained, and the resin was washed sequentially with *N,N*-dimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The resin was treated with 3.8 ml of 2.0 M SnCl₂•dihydrate in *N*-methylpyrrolidinone solution and rotated at 25°C for 24 hours. The reaction was drained and the resin washed sequentially with 30% ethylenediamine (3X), *N,N*-dimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The dried diamine resin was treated with 7.6 ml of a 0.5 M benzyhydryl isothiocyanate in *N*-methylpyrrolidinone solution and 7.6 ml of a 1.0 M diisopropylcarbodiimide in *N*-methylpyrrolidinone solution. After rotating at 80°C for 24 h the reaction was cooled to 25°C, drained, and the resin was washed sequentially with *N,N*-dimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The resin was treated with 30 ml 95% trifluoroacetic acid (TFA) in water and rotated at 25°C for 3 hours. The resin was drained and washed with dichloromethane. The filtrate was concentrated *in vacuo* to give an oil. The oil was redissolved in dichloromethane and the solution was washed twice with saturated sodium bicarbonate (NaHCO₃). The organic layer was dried (Na₂SO₄), filtered, and concentrated *in vacuo*. The crude

-130-

product was triturated with Et₂O/hexanes, and the solid was collected by filtration to give 333 mg (98% yield) of the title compound as an off-white solid:

¹H NMR (DMSO-*d*₆, 400 MHz) δ 7.68 (m, 2 H), 7.63 (d, 1 H, J = 8.4), 7.54 (dd, 1 H, J = 8.0, 1.2), 7.40-7.00 (m, 17 H), 6.36 (d, 1 H, J = 8), 4.42 (t, 2 H, J = 7.4), 2.97 (t, 2 H, J = 7.4); MS (ESP+) *m/e* 447 (MH⁺).

Table 2
Atomic Structure Coordinate Data Obtained From
X-ray Diffraction From the Ligand-binding Domain of CAR
In Complex With Compound 1

10

15

20

25

30

35

40

45

ATOM	1	N	LEU A 120	34.417	18.787	67.312	1.00	50.31	N
ATOM	2	CA	LEU A 120	34.298	17.304	67.212	1.00	49.96	C
ATOM	3	C	LEU A 120	33.672	16.891	65.886	1.00	49.44	C
ATOM	4	O	LEU A 120	32.815	17.592	65.344	1.00	49.49	O
ATOM	5	CB	LEU A 120	33.447	16.756	68.363	1.00	50.64	C
ATOM	6	CG	LEU A 120	34.003	16.880	69.783	1.00	51.38	C
ATOM	7	CD1	LEU A 120	32.969	16.374	70.777	1.00	51.56	C
ATOM	8	CD2	LEU A 120	35.297	16.085	69.906	1.00	51.43	C
ATOM	9	N	ARG A 121	34.106	15.745	65.375	1.00	48.14	N
ATOM	10	CA	ARG A 121	33.599	15.221	64.117	1.00	47.01	C
ATOM	11	C	ARG A 121	33.113	13.790	64.314	1.00	45.50	C
ATOM	12	O	ARG A 121	33.775	12.836	63.905	1.00	45.36	O
ATOM	13	CB	ARG A 121	34.700	15.264	63.052	1.00	48.45	C
ATOM	14	CG	ARG A 121	35.233	16.664	62.790	1.00	49.89	C
ATOM	15	CD	ARG A 121	36.430	16.655	61.852	1.00	52.32	C
ATOM	16	NE	ARG A 121	36.100	16.133	60.529	1.00	53.49	N
ATOM	17	CZ	ARG A 121	36.947	16.112	59.504	1.00	54.08	C
ATOM	18	NH1	ARG A 121	38.178	16.586	59.648	1.00	54.50	N
ATOM	19	NH2	ARG A 121	36.563	15.620	58.334	1.00	54.12	N
ATOM	20	N	PRO A 122	31.946	13.622	64.955	1.00	43.87	N
ATOM	21	CA	PRO A 122	31.403	12.282	65.187	1.00	42.99	C
ATOM	22	C	PRO A 122	31.173	11.529	63.881	1.00	42.25	C
ATOM	23	O	PRO A 122	30.823	12.125	62.862	1.00	42.01	O
ATOM	24	CB	PRO A 122	30.105	12.561	65.944	1.00	42.59	C
ATOM	25	CG	PRO A 122	29.699	13.908	65.437	1.00	43.60	C
ATOM	26	CD	PRO A 122	31.010	14.655	65.429	1.00	43.27	C
ATOM	27	N	LYS A 123	31.379	10.218	63.920	1.00	41.53	N
ATOM	28	CA	LYS A 123	31.205	9.378	62.744	1.00	41.30	C
ATOM	29	C	LYS A 123	29.732	9.158	62.431	1.00	40.35	C
ATOM	30	O	LYS A 123	28.877	9.250	63.313	1.00	39.21	O
ATOM	31	CB	LYS A 123	31.885	8.024	62.965	1.00	42.56	C
ATOM	32	CG	LYS A 123	33.371	8.127	63.279	1.00	45.26	C
ATOM	33	CD	LYS A 123	33.979	6.761	63.564	1.00	46.98	C
ATOM	34	CE	LYS A 123	35.463	6.876	63.882	1.00	47.93	C
ATOM	35	NZ	LYS A 123	36.066	5.558	64.225	1.00	49.23	N
ATOM	36	N	LEU A 124	29.439	8.879	61.165	1.00	39.48	N
ATOM	37	CA	LEU A 124	28.071	8.622	60.744	1.00	38.64	C
ATOM	38	C	LEU A 124	27.606	7.325	61.384	1.00	38.41	C

-131-

	ATOM	39	O	LEU	A	124	28.293	6.308	61.304	1.00	39.12	O
	ATOM	40	CB	LEU	A	124	27.996	8.491	59.220	1.00	37.76	C
	ATOM	41	CG	LEU	A	124	28.162	9.776	58.406	1.00	37.83	C
5	ATOM	42	CD1	LEU	A	124	28.401	9.438	56.941	1.00	37.98	C
	ATOM	43	CD2	LEU	A	124	26.922	10.633	58.564	1.00	36.97	C
	ATOM	44	N	SER	A	125	26.448	7.362	62.029	1.00	38.47	N
	ATOM	45	CA	SER	A	125	25.905	6.168	62.661	1.00	39.40	C
	ATOM	46	C	SER	A	125	25.496	5.197	61.561	1.00	40.52	C
10	ATOM	47	O	SER	A	125	25.386	5.581	60.395	1.00	39.53	O
	ATOM	48	CB	SER	A	125	24.679	6.523	63.495	1.00	39.88	C
	ATOM	49	OG	SER	A	125	23.619	6.951	62.660	1.00	40.18	O
	ATOM	50	N	GLU	A	126	25.271	3.940	61.923	1.00	41.33	N
	ATOM	51	CA	GLU	A	126	24.865	2.956	60.930	1.00	42.41	C
15	ATOM	52	C	GLU	A	126	23.535	3.385	60.314	1.00	41.49	C
	ATOM	53	O	GLU	A	126	23.313	3.207	59.115	1.00	41.40	O
	ATOM	54	CB	GLU	A	126	24.727	1.573	61.573	1.00	45.02	C
	ATOM	55	CG	GLU	A	126	24.325	0.463	60.605	1.00	48.95	C
	ATOM	56	CD	GLU	A	126	25.202	0.414	59.361	1.00	51.93	C
20	ATOM	57	OE1	GLU	A	126	24.878	1.105	58.366	1.00	53.34	O
	ATOM	58	OE2	GLU	A	126	26.222	-0.308	59.379	1.00	53.64	O
	ATOM	59	N	GLU	A	127	22.659	3.960	61.133	1.00	40.27	N
	ATOM	60	CA	GLU	A	127	21.358	4.412	60.650	1.00	39.52	C
	ATOM	61	C	GLU	A	127	21.512	5.550	59.647	1.00	37.38	C
25	ATOM	62	O	GLU	A	127	20.814	5.594	58.630	1.00	36.24	O
	ATOM	63	CB	GLU	A	127	20.481	4.891	61.807	1.00	41.53	C
	ATOM	64	CG	GLU	A	127	19.091	5.320	61.363	1.00	45.78	C
	ATOM	65	CD	GLU	A	127	18.236	5.832	62.504	1.00	47.87	C
	ATOM	66	OE1	GLU	A	127	18.572	6.890	63.075	1.00	49.93	O
30	ATOM	67	OE2	GLU	A	127	17.227	5.173	62.832	1.00	50.45	O
	ATOM	68	N	GLN	A	128	22.420	6.473	59.939	1.00	34.92	N
	ATOM	69	CA	GLN	A	128	22.654	7.603	59.052	1.00	33.94	C
	ATOM	70	C	GLN	A	128	23.239	7.134	57.721	1.00	34.19	C
	ATOM	71	O	GLN	A	128	22.905	7.671	56.665	1.00	32.45	O
35	ATOM	72	CB	GLN	A	128	23.573	8.622	59.735	1.00	33.20	C
	ATOM	73	CG	GLN	A	128	22.861	9.410	60.835	1.00	32.00	C
	ATOM	74	CD	GLN	A	128	23.785	10.317	61.629	1.00	32.20	C
	ATOM	75	OE1	GLN	A	128	23.346	11.326	62.192	1.00	33.66	O
	ATOM	76	NE2	GLN	A	128	25.061	9.960	61.691	1.00	30.80	N
40	ATOM	77	N	GLN	A	129	24.101	6.124	57.768	1.00	33.75	N
	ATOM	78	CA	GLN	A	129	24.692	5.591	56.545	1.00	35.00	C
	ATOM	79	C	GLN	A	129	23.588	4.965	55.702	1.00	34.31	C
	ATOM	80	O	GLN	A	129	23.562	5.111	54.479	1.00	33.78	O
	ATOM	81	CB	GLN	A	129	25.747	4.531	56.874	1.00	37.89	C
45	ATOM	82	CG	GLN	A	129	26.977	5.078	57.579	1.00	42.41	C
	ATOM	83	CD	GLN	A	129	27.983	3.995	57.929	1.00	45.15	C
	ATOM	84	OE1	GLN	A	129	28.998	4.261	58.575	1.00	46.46	O
	ATOM	85	NE2	GLN	A	129	27.704	2.766	57.504	1.00	46.27	N
	ATOM	86	N	ARG	A	130	22.674	4.270	56.370	1.00	33.44	N
50	ATOM	87	CA	ARG	A	130	21.556	3.614	55.703	1.00	34.05	C
	ATOM	88	C	ARG	A	130	20.653	4.638	55.018	1.00	32.98	C
	ATOM	89	O	ARG	A	130	20.226	4.436	53.881	1.00	31.44	O
	ATOM	90	CB	ARG	A	130	20.759	2.794	56.723	1.00	37.04	C
	ATOM	91	CG	ARG	A	130	19.497	2.141	56.184	1.00	41.36	C
55	ATOM	92	CD	ARG	A	130	18.961	1.108	57.171	1.00	45.69	C
	ATOM	93	NE	ARG	A	130	17.642	0.608	56.790	1.00	49.25	N
	ATOM	94	CZ	ARG	A	130	16.510	1.291	56.938	1.00	51.46	C
	ATOM	95	NH1	ARG	A	130	16.529	2.510	57.465	1.00	52.76	N
	ATOM	96	NH2	ARG	A	130	15.357	0.757	56.556	1.00	52.73	N

-132-

	ATOM	97	N	ILE A 131	20.367	5.735	55.712	1.00	31.16	N
	ATOM	98	CA	ILE A 131	19.519	6.790	55.158	1.00	30.41	C
	ATOM	99	C	ILE A 131	20.120	7.343	53.865	1.00	29.21	C
5	ATOM	100	O	ILE A 131	19.414	7.528	52.872	1.00	27.86	O
	ATOM	101	CB	ILE A 131	19.334	7.945	56.177	1.00	31.61	C
	ATOM	102	CG1	ILE A 131	18.513	7.448	57.372	1.00	32.47	C
	ATOM	103	CG2	ILE A 131	18.657	9.138	55.507	1.00	31.13	C
	ATOM	104	CD1	ILE A 131	18.287	8.496	58.457	1.00	33.63	C
10	ATOM	105	N	ILE A 132	21.424	7.601	53.876	1.00	28.81	N
	ATOM	106	CA	ILE A 132	22.094	8.124	52.691	1.00	29.13	C
	ATOM	107	C	ILE A 132	22.029	7.115	51.544	1.00	29.37	C
	ATOM	108	O	ILE A 132	21.786	7.486	50.394	1.00	28.72	O
	ATOM	109	CB	ILE A 132	23.570	8.468	52.994	1.00	29.90	C
15	ATOM	110	CG1	ILE A 132	23.628	9.625	53.995	1.00	30.31	C
	ATOM	111	CG2	ILE A 132	24.306	8.838	51.708	1.00	30.32	C
	ATOM	112	CD1	ILE A 132	25.027	9.997	54.432	1.00	31.33	C
	ATOM	113	N	ALA A 133	22.239	5.841	51.862	1.00	28.31	N
	ATOM	114	CA	ALA A 133	22.203	4.785	50.851	1.00	27.51	C
20	ATOM	115	C	ALA A 133	20.820	4.680	50.213	1.00	26.94	C
	ATOM	116	O	ALA A 133	20.694	4.542	48.993	1.00	26.91	O
	ATOM	117	CB	ALA A 133	22.587	3.454	51.479	1.00	27.94	C
	ATOM	118	N	ILE A 134	19.786	4.739	51.044	1.00	26.00	N
	ATOM	119	CA	ILE A 134	18.413	4.659	50.564	1.00	25.19	C
25	ATOM	120	C	ILE A 134	18.090	5.832	49.643	1.00	24.84	C
	ATOM	121	O	ILE A 134	17.490	5.651	48.585	1.00	23.10	O
	ATOM	122	CB	ILE A 134	17.416	4.660	51.742	1.00	26.47	C
	ATOM	123	CG1	ILE A 134	17.511	3.331	52.493	1.00	27.92	C
	ATOM	124	CG2	ILE A 134	15.997	4.901	51.239	1.00	26.56	C
30	ATOM	125	CD1	ILE A 134	16.714	3.297	53.778	1.00	29.71	C
	ATOM	126	N	LEU A 135	18.494	7.030	50.047	1.00	23.54	N
	ATOM	127	CA	LEU A 135	18.228	8.220	49.242	1.00	23.28	C
	ATOM	128	C	LEU A 135	18.987	8.217	47.914	1.00	22.05	C
	ATOM	129	O	LEU A 135	18.454	8.656	46.894	1.00	21.44	O
35	ATOM	130	CB	LEU A 135	18.559	9.480	50.045	1.00	23.21	C
	ATOM	131	CG	LEU A 135	17.644	9.754	51.246	1.00	24.57	C
	ATOM	132	CD1	LEU A 135	18.057	11.076	51.900	1.00	26.44	C
	ATOM	133	CD2	LEU A 135	16.185	9.820	50.789	1.00	25.56	C
	ATOM	134	N	LEU A 136	20.223	7.725	47.913	1.00	22.40	N
40	ATOM	135	CA	LEU A 136	20.991	7.675	46.669	1.00	23.29	C
	ATOM	136	C	LEU A 136	20.302	6.721	45.705	1.00	23.50	C
	ATOM	137	O	LEU A 136	20.191	6.996	44.512	1.00	23.31	O
	ATOM	138	CB	LEU A 136	22.424	7.194	46.920	1.00	24.60	C
	ATOM	139	CG	LEU A 136	23.395	8.196	47.549	1.00	25.56	C
45	ATOM	140	CD1	LEU A 136	24.740	7.518	47.798	1.00	26.67	C
	ATOM	141	CD2	LEU A 136	23.555	9.398	46.628	1.00	26.04	C
	ATOM	142	N	ASP A 137	19.845	5.591	46.232	1.00	23.87	N
	ATOM	143	CA	ASP A 137	19.156	4.589	45.427	1.00	23.95	C
	ATOM	144	C	ASP A 137	17.844	5.152	44.870	1.00	23.67	C
50	ATOM	145	O	ASP A 137	17.513	4.943	43.697	1.00	22.79	O
	ATOM	146	CB	ASP A 137	18.886	3.348	46.282	1.00	26.93	C
	ATOM	147	CG	ASP A 137	18.158	2.266	45.524	1.00	31.10	C
	ATOM	148	OD1	ASP A 137	17.010	1.947	45.900	1.00	34.78	O
	ATOM	149	OD2	ASP A 137	18.730	1.734	44.552	1.00	34.13	O
55	ATOM	150	N	ALA A 138	17.105	5.867	45.714	1.00	22.31	N
	ATOM	151	CA	ALA A 138	15.836	6.472	45.312	1.00	22.31	C
	ATOM	152	C	ALA A 138	16.063	7.435	44.157	1.00	21.39	C
	ATOM	153	O	ALA A 138	15.310	7.445	43.183	1.00	20.83	O
	ATOM	154	CB	ALA A 138	15.213	7.219	46.487	1.00	23.04	C

-133-

	ATOM	155	N	HIS	A	139	17.107	8.249	44.263	1.00	21.06	N
	ATOM	156	CA	HIS	A	139	17.408	9.202	43.208	1.00	21.28	C
	ATOM	157	C	HIS	A	139	17.814	8.511	41.905	1.00	21.64	C
5	ATOM	158	O	HIS	A	139	17.385	8.913	40.824	1.00	21.17	O
	ATOM	159	CB	HIS	A	139	18.528	10.152	43.631	1.00	21.21	C
	ATOM	160	CG	HIS	A	139	18.730	11.288	42.680	1.00	22.53	C
	ATOM	161	ND1	HIS	A	139	19.955	11.593	42.126	1.00	25.49	N
	ATOM	162	CD2	HIS	A	139	17.850	12.173	42.157	1.00	19.49	C
10	ATOM	163	CE1	HIS	A	139	19.820	12.615	41.300	1.00	20.82	C
	ATOM	164	NE2	HIS	A	139	18.552	12.986	41.301	1.00	23.99	N
	ATOM	165	N	HIS	A	140	18.650	7.479	42.005	1.00	21.50	N
	ATOM	166	CA	HIS	A	140	19.099	6.760	40.819	1.00	22.20	C
	ATOM	167	C	HIS	A	140	17.947	6.088	40.082	1.00	21.95	C
15	ATOM	168	O	HIS	A	140	17.997	5.911	38.861	1.00	21.87	O
	ATOM	169	CB	HIS	A	140	20.153	5.710	41.193	1.00	23.76	C
	ATOM	170	CG	HIS	A	140	21.398	6.291	41.787	1.00	25.80	C
	ATOM	171	ND1	HIS	A	140	21.803	7.585	41.546	1.00	27.26	N
	ATOM	172	CD2	HIS	A	140	22.341	5.745	42.591	1.00	26.22	C
20	ATOM	173	CE1	HIS	A	140	22.942	7.814	42.176	1.00	26.08	C
	ATOM	174	NE2	HIS	A	140	23.291	6.714	42.817	1.00	27.71	N
	ATOM	175	N	LYS	A	141	16.908	5.719	40.821	1.00	20.41	N
	ATOM	176	CA	LYS	A	141	15.745	5.071	40.225	1.00	21.89	C
	ATOM	177	C	LYS	A	141	14.746	6.078	39.665	1.00	21.31	C
25	ATOM	178	O	LYS	A	141	13.916	5.730	38.832	1.00	22.47	O
	ATOM	179	CB	LYS	A	141	15.031	4.203	41.265	1.00	23.28	C
	ATOM	180	CG	LYS	A	141	15.804	2.960	41.668	1.00	26.83	C
	ATOM	181	CD	LYS	A	141	15.080	2.209	42.771	1.00	30.63	C
	ATOM	182	CE	LYS	A	141	15.781	0.902	43.093	1.00	33.64	C
30	ATOM	183	NZ	LYS	A	141	15.122	0.206	44.231	1.00	36.58	N
	ATOM	184	N	THR	A	142	14.840	7.325	40.107	1.00	20.65	N
	ATOM	185	CA	THR	A	142	13.893	8.348	39.664	1.00	20.68	C
	ATOM	186	C	THR	A	142	14.440	9.502	38.833	1.00	20.45	C
	ATOM	187	O	THR	A	142	13.682	10.375	38.420	1.00	20.32	O
35	ATOM	188	CB	THR	A	142	13.142	8.935	40.865	1.00	20.48	C
	ATOM	189	OG1	THR	A	142	14.081	9.474	41.805	1.00	18.91	O
	ATOM	190	CG2	THR	A	142	12.326	7.850	41.546	1.00	19.94	C
	ATOM	191	N	TYR	A	143	15.747	9.520	38.595	1.00	20.03	N
	ATOM	192	CA	TYR	A	143	16.342	10.566	37.768	1.00	20.44	C
40	ATOM	193	C	TYR	A	143	17.207	9.895	36.706	1.00	20.75	C
	ATOM	194	O	TYR	A	143	18.248	9.323	37.013	1.00	21.56	O
	ATOM	195	CB	TYR	A	143	17.198	11.529	38.610	1.00	20.88	C
	ATOM	196	CG	TYR	A	143	17.673	12.742	37.835	1.00	20.90	C
	ATOM	197	CD1	TYR	A	143	18.721	12.650	36.915	1.00	21.44	C
45	ATOM	198	CD2	TYR	A	143	17.048	13.980	37.994	1.00	21.13	C
	ATOM	199	CE1	TYR	A	143	19.132	13.762	36.170	1.00	21.80	C
	ATOM	200	CE2	TYR	A	143	17.449	15.090	37.253	1.00	20.26	C
	ATOM	201	CZ	TYR	A	143	18.487	14.978	36.347	1.00	22.15	C
	ATOM	202	OH	TYR	A	143	18.868	16.077	35.612	1.00	21.28	O
50	ATOM	203	N	ASP	A	144	16.750	9.959	35.461	1.00	20.48	N
	ATOM	204	CA	ASP	A	144	17.449	9.365	34.326	1.00	21.36	C
	ATOM	205	C	ASP	A	144	18.428	10.387	33.751	1.00	22.06	C
	ATOM	206	O	ASP	A	144	18.016	11.348	33.102	1.00	21.75	O
	ATOM	207	CB	ASP	A	144	16.412	8.955	33.274	1.00	21.65	C
	ATOM	208	CG	ASP	A	144	17.032	8.481	31.976	1.00	22.22	C
55	ATOM	209	OD1	ASP	A	144	18.261	8.286	31.921	1.00	22.12	O
	ATOM	210	OD2	ASP	A	144	16.266	8.294	31.007	1.00	23.20	O
	ATOM	211	N	PRO	A	145	19.741	10.183	33.976	1.00	21.93	N
	ATOM	212	CA	PRO	A	145	20.779	11.094	33.483	1.00	23.05	C

-134-

	ATOM	213	C	PRO A 145	20.968	11.106	31.968	1.00	22.50	C
	ATOM	214	O	PRO A 145	21.754	11.906	31.451	1.00	23.61	O
	ATOM	215	CB	PRO A 145	22.026	10.620	34.225	1.00	23.45	C
5	ATOM	216	CG	PRO A 145	21.809	9.150	34.297	1.00	24.95	C
	ATOM	217	CD	PRO A 145	20.347	9.052	34.700	1.00	23.26	C
	ATOM	218	N	THR A 146	20.265	10.224	31.256	1.00	22.03	N
	ATOM	219	CA	THR A 146	20.364	10.192	29.796	1.00	21.95	C
	ATOM	220	C	THR A 146	19.174	10.907	29.155	1.00	22.52	C
10	ATOM	221	O	THR A 146	19.181	11.177	27.953	1.00	22.17	O
	ATOM	222	CB	THR A 146	20.433	8.750	29.233	1.00	21.96	C
	ATOM	223	OG1	THR A 146	19.167	8.099	29.395	1.00	21.08	O
	ATOM	224	CG2	THR A 146	21.509	7.949	29.956	1.00	23.14	C
	ATOM	225	N	TYR A 147	18.158	11.210	29.963	1.00	22.04	N
15	ATOM	226	CA	TYR A 147	16.963	11.912	29.489	1.00	22.53	C
	ATOM	227	C	TYR A 147	16.313	11.191	28.309	1.00	23.10	C
	ATOM	228	O	TYR A 147	15.789	11.821	27.393	1.00	23.05	O
	ATOM	229	CB	TYR A 147	17.335	13.350	29.093	1.00	23.34	C
	ATOM	230	CG	TYR A 147	18.159	14.049	30.150	1.00	23.73	C
20	ATOM	231	CD1	TYR A 147	19.525	14.274	29.968	1.00	25.15	C
	ATOM	232	CD2	TYR A 147	17.593	14.398	31.372	1.00	23.61	C
	ATOM	233	CE1	TYR A 147	20.304	14.818	30.989	1.00	25.82	C
	ATOM	234	CE2	TYR A 147	18.363	14.941	32.396	1.00	26.56	C
	ATOM	235	CZ	TYR A 147	19.716	15.142	32.199	1.00	26.11	C
25	ATOM	236	OH	TYR A 147	20.484	15.619	33.237	1.00	29.64	O
	ATOM	237	N	SER A 148	16.326	9.862	28.355	1.00	23.29	N
	ATOM	238	CA	SER A 148	15.781	9.046	27.278	1.00	23.65	C
	ATOM	239	C	SER A 148	14.263	9.078	27.073	1.00	24.65	C
	ATOM	240	O	SER A 148	13.783	8.650	26.024	1.00	24.62	O
30	ATOM	241	CB	SER A 148	16.243	7.593	27.450	1.00	26.66	C
	ATOM	242	OG	SER A 148	15.684	7.006	28.614	1.00	29.82	O
	ATOM	243	N	ASP A 149	13.505	9.576	28.048	1.00	22.99	N
	ATOM	244	CA	ASP A 149	12.045	9.632	27.905	1.00	23.85	C
	ATOM	245	C	ASP A 149	11.534	10.925	27.272	1.00	24.00	C
35	ATOM	246	O	ASP A 149	10.371	11.008	26.879	1.00	24.41	O
	ATOM	247	CB	ASP A 149	11.349	9.488	29.263	1.00	24.47	C
	ATOM	248	CG	ASP A 149	11.517	8.114	29.872	1.00	27.05	C
	ATOM	249	OD1	ASP A 149	11.441	7.116	29.124	1.00	26.86	O
	ATOM	250	OD2	ASP A 149	11.707	8.037	31.105	1.00	26.29	O
40	ATOM	251	N	PHE A 150	12.396	11.927	27.171	1.00	24.31	N
	ATOM	252	CA	PHE A 150	11.995	13.231	26.646	1.00	25.09	C
	ATOM	253	C	PHE A 150	11.363	13.263	25.252	1.00	25.91	C
	ATOM	254	O	PHE A 150	10.565	14.155	24.949	1.00	25.61	O
	ATOM	255	CB	PHE A 150	13.188	14.187	26.715	1.00	24.68	C
45	ATOM	256	CG	PHE A 150	13.546	14.611	28.121	1.00	25.17	C
	ATOM	257	CD1	PHE A 150	13.422	13.726	29.187	1.00	25.54	C
	ATOM	258	CD2	PHE A 150	14.028	15.891	28.374	1.00	26.43	C
	ATOM	259	CE1	PHE A 150	13.773	14.104	30.484	1.00	25.74	C
	ATOM	260	CE2	PHE A 150	14.384	16.278	29.667	1.00	25.55	C
50	ATOM	261	CZ	PHE A 150	14.256	15.386	30.721	1.00	24.63	C
	ATOM	262	N	CYS A 151	11.694	12.298	24.404	1.00	27.60	N
	ATOM	263	CA	CYS A 151	11.116	12.286	23.063	1.00	28.74	C
	ATOM	264	C	CYS A 151	9.640	11.891	23.094	1.00	28.90	C
	ATOM	265	O	CYS A 151	8.951	11.958	22.075	1.00	28.40	O
55	ATOM	266	CB	CYS A 151	11.894	11.332	22.154	1.00	31.34	C
	ATOM	267	SG	CYS A 151	11.886	9.633	22.716	1.00	37.88	S
	ATOM	268	N	GLN A 152	9.152	11.482	24.262	1.00	27.55	N
	ATOM	269	CA	GLN A 152	7.753	11.093	24.393	1.00	27.93	C
	ATOM	270	C	GLN A 152	6.858	12.285	24.711	1.00	27.73	C

-135-

	ATOM	271	O	GLN A 152	5.633	12.202	24.590	1.00	28.51	O
	ATOM	272	CB	GLN A 152	7.602	10.021	25.473	1.00	29.61	C
	ATOM	273	CG	GLN A 152	8.312	8.724	25.123	1.00	33.35	C
5	ATOM	274	CD	GLN A 152	8.121	7.650	26.173	1.00	36.62	C
	ATOM	275	OE1	GLN A 152	6.995	7.260	26.478	1.00	39.37	O
	ATOM	276	NE2	GLN A 152	9.225	7.162	26.732	1.00	38.35	N
	ATOM	277	N	PHE A 153	7.469	13.395	25.115	1.00	25.45	N
	ATOM	278	CA	PHE A 153	6.705	14.597	25.439	1.00	25.30	C
10	ATOM	279	C	PHE A 153	6.261	15.273	24.151	1.00	25.61	C
	ATOM	280	O	PHE A 153	6.799	14.998	23.071	1.00	24.69	O
	ATOM	281	CB	PHE A 153	7.564	15.608	26.215	1.00	23.94	C
	ATOM	282	CG	PHE A 153	8.187	15.060	27.469	1.00	23.45	C
	ATOM	283	CD1	PHE A 153	9.332	15.654	27.990	1.00	22.75	C
15	ATOM	284	CD2	PHE A 153	7.654	13.949	28.116	1.00	23.40	C
	ATOM	285	CE1	PHE A 153	9.948	15.146	29.133	1.00	23.18	C
	ATOM	286	CE2	PHE A 153	8.261	13.434	29.263	1.00	22.50	C
	ATOM	287	CZ	PHE A 153	9.414	14.037	29.769	1.00	22.91	C
	ATOM	288	N	ARG A 154	5.276	16.158	24.260	1.00	25.51	N
20	ATOM	289	CA	ARG A 154	4.842	16.902	23.092	1.00	26.08	C
	ATOM	290	C	ARG A 154	6.094	17.673	22.689	1.00	27.20	C
	ATOM	291	O	ARG A 154	6.824	18.184	23.542	1.00	26.99	O
	ATOM	292	CB	ARG A 154	3.681	17.830	23.449	1.00	26.73	C
	ATOM	293	CG	ARG A 154	2.351	17.087	23.522	1.00	27.85	C
25	ATOM	294	CD	ARG A 154	1.232	17.964	24.066	1.00	27.71	C
	ATOM	295	NE	ARG A 154	1.347	18.138	25.509	1.00	27.14	N
	ATOM	296	CZ	ARG A 154	0.497	18.839	26.248	1.00	28.47	C
	ATOM	297	NH1	ARG A 154	-0.538	19.444	25.677	1.00	29.16	N
	ATOM	298	NH2	ARG A 154	0.673	18.919	27.560	1.00	27.66	N
30	ATOM	299	N	PRO A 155	6.368	17.757	21.384	1.00	27.28	N
	ATOM	300	CA	PRO A 155	7.554	18.454	20.892	1.00	28.12	C
	ATOM	301	C	PRO A 155	7.709	19.929	21.217	1.00	28.41	C
	ATOM	302	O	PRO A 155	6.733	20.676	21.291	1.00	27.77	O
	ATOM	303	CB	PRO A 155	7.491	18.206	19.388	1.00	28.83	C
35	ATOM	304	CG	PRO A 155	6.020	18.191	19.130	1.00	29.19	C
	ATOM	305	CD	PRO A 155	5.508	17.335	20.262	1.00	28.61	C
	ATOM	306	N	PRO A 156	8.956	20.361	21.437	1.00	28.25	N
	ATOM	307	CA	PRO A 156	9.202	21.768	21.739	1.00	29.56	C
	ATOM	308	C	PRO A 156	9.054	22.532	20.425	1.00	30.08	C
40	ATOM	309	O	PRO A 156	9.483	22.054	19.371	1.00	30.96	O
	ATOM	310	CB	PRO A 156	10.640	21.763	22.250	1.00	29.92	C
	ATOM	311	CG	PRO A 156	11.262	20.646	21.476	1.00	30.45	C
	ATOM	312	CD	PRO A 156	10.198	19.573	21.538	1.00	29.15	C
	ATOM	313	N	VAL A 157	8.417	23.693	20.489	1.00	30.75	N
45	ATOM	314	CA	VAL A 157	8.220	24.538	19.319	1.00	31.52	C
	ATOM	315	C	VAL A 157	8.764	25.907	19.692	1.00	32.33	C
	ATOM	316	O	VAL A 157	8.361	26.482	20.698	1.00	33.09	O
	ATOM	317	CB	VAL A 157	6.727	24.663	18.962	1.00	31.97	C
	ATOM	318	CG1	VAL A 157	6.544	25.654	17.825	1.00	32.48	C
50	ATOM	319	CG2	VAL A 157	6.177	23.302	18.573	1.00	32.24	C
	ATOM	320	N	ARG A 158	9.681	26.425	18.885	1.00	33.83	N
	ATOM	321	CA	ARG A 158	10.289	27.716	19.173	1.00	36.19	C
	ATOM	322	C	ARG A 158	10.020	28.766	18.096	1.00	38.44	C
	ATOM	323	O	ARG A 158	10.763	28.881	17.123	1.00	39.20	O
55	ATOM	324	CB	ARG A 158	11.794	27.523	19.367	1.00	35.86	C
	ATOM	325	CG	ARG A 158	12.131	26.585	20.524	1.00	34.74	C
	ATOM	326	CD	ARG A 158	13.606	26.231	20.561	1.00	35.06	C
	ATOM	327	NE	ARG A 158	13.991	25.641	21.841	1.00	32.63	N
	ATOM	328	CZ	ARG A 158	14.006	24.339	22.113	1.00	31.82	C

-136-

	ATOM	329	NH1	ARG	A	158	13.658	23.450	21.192	1.00	32.10	N
	ATOM	330	NH2	ARG	A	158	14.370	23.926	23.319	1.00	29.69	N
	ATOM	331	N	VAL	A	159	8.949	29.531	18.284	1.00	40.67	N
5	ATOM	332	CA	VAL	A	159	8.568	30.574	17.338	1.00	42.44	C
	ATOM	333	C	VAL	A	159	9.511	31.767	17.432	1.00	43.24	C
	ATOM	334	O	VAL	A	159	10.170	31.968	18.451	1.00	42.85	O
	ATOM	335	CB	VAL	A	159	7.135	31.066	17.607	1.00	42.85	C
	ATOM	336	CG1	VAL	A	159	6.147	29.937	17.367	1.00	43.48	C
10	ATOM	337	CG2	VAL	A	159	7.027	31.577	19.040	1.00	43.60	C
	ATOM	338	N	ASN	A	160	9.576	32.557	16.365	1.00	44.06	N
	ATOM	339	CA	ASN	A	160	10.440	33.730	16.357	1.00	44.92	C
	ATOM	340	C	ASN	A	160	9.876	34.768	17.320	1.00	45.24	C
	ATOM	341	O	ASN	A	160	8.728	35.198	17.185	1.00	45.27	O
15	ATOM	342	CB	ASN	A	160	10.530	34.326	14.949	1.00	46.00	C
	ATOM	343	CG	ASN	A	160	11.017	33.322	13.921	1.00	47.25	C
	ATOM	344	OD1	ASN	A	160	12.030	32.649	14.124	1.00	47.25	O
	ATOM	345	ND2	ASN	A	160	10.298	33.218	12.808	1.00	48.36	N
	ATOM	346	N	ASP	A	161	10.688	35.156	18.298	1.00	45.02	N
20	ATOM	347	CA	ASP	A	161	10.282	36.142	19.289	1.00	44.79	C
	ATOM	348	C	ASP	A	161	11.515	36.834	19.862	1.00	44.74	C
	ATOM	349	O	ASP	A	161	11.679	36.939	21.077	1.00	44.64	O
	ATOM	350	CB	ASP	A	161	9.483	35.463	20.406	1.00	44.26	C
	ATOM	351	CG	ASP	A	161	9.101	36.421	21.515	1.00	44.34	C
25	ATOM	352	OD1	ASP	A	161	8.640	37.540	21.201	1.00	43.26	O
	ATOM	353	OD2	ASP	A	161	9.258	36.054	22.700	1.00	43.90	O
	ATOM	354	N	GLY	A	162	12.383	37.304	18.972	1.00	44.73	N
	ATOM	355	CA	GLY	A	162	13.592	37.977	19.409	1.00	44.74	C
	ATOM	356	C	GLY	A	162	13.292	39.196	20.261	1.00	44.56	C
30	ATOM	357	O	GLY	A	162	14.135	39.638	21.042	1.00	45.10	O
	ATOM	358	N	GLY	A	163	12.086	39.736	20.116	1.00	44.30	N
	ATOM	359	CA	GLY	A	163	11.706	40.911	20.879	1.00	43.74	C
	ATOM	360	C	GLY	A	163	11.206	40.618	22.282	1.00	43.23	C
	ATOM	361	O	GLY	A	163	11.066	41.533	23.096	1.00	43.53	O
35	ATOM	362	N	GLY	A	164	10.946	39.346	22.572	1.00	42.43	N
	ATOM	363	CA	GLY	A	164	10.450	38.980	23.889	1.00	40.70	C
	ATOM	364	C	GLY	A	164	9.094	39.616	24.130	1.00	39.47	C
	ATOM	365	O	GLY	A	164	8.812	40.125	25.222	1.00	40.10	O
	ATOM	366	N	SER	A	216	8.256	39.587	23.099	1.00	36.82	N
40	ATOM	367	CA	SER	A	216	6.918	40.165	23.162	1.00	35.37	C
	ATOM	368	C	SER	A	216	5.965	39.359	24.032	1.00	34.15	C
	ATOM	369	O	SER	A	216	5.653	38.213	23.721	1.00	32.50	O
	ATOM	370	CB	SER	A	216	6.329	40.277	21.755	1.00	35.39	C
	ATOM	371	OG	SER	A	216	4.958	40.634	21.812	1.00	35.41	O
45	ATOM	372	N	VAL	A	217	5.495	39.969	25.116	1.00	33.39	N
	ATOM	373	CA	VAL	A	217	4.563	39.301	26.013	1.00	33.22	C
	ATOM	374	C	VAL	A	217	3.299	38.922	25.251	1.00	32.19	C
	ATOM	375	O	VAL	A	217	2.783	37.816	25.399	1.00	31.92	O
	ATOM	376	CB	VAL	A	217	4.161	40.208	27.195	1.00	33.21	C
	ATOM	377	CG1	VAL	A	217	3.203	39.462	28.119	1.00	35.52	C
50	ATOM	378	CG2	VAL	A	217	5.396	40.644	27.960	1.00	35.70	C
	ATOM	379	N	THR	A	218	2.809	39.846	24.428	1.00	31.30	N
	ATOM	380	CA	THR	A	218	1.597	39.609	23.653	1.00	30.58	C
	ATOM	381	C	THR	A	218	1.736	38.398	22.741	1.00	30.30	C
55	ATOM	382	O	THR	A	218	0.852	37.544	22.695	1.00	30.29	O
	ATOM	383	CB	THR	A	218	1.235	40.843	22.802	1.00	30.65	C
	ATOM	384	OG1	THR	A	218	1.025	41.966	23.667	1.00	30.30	O
	ATOM	385	CG2	THR	A	218	-0.035	40.587	22.000	1.00	31.23	C
	ATOM	386	N	LEU	A	219	2.849	38.325	22.018	1.00	29.44	N

-137-

	ATOM	387	CA	LEU A 219	3.095	37.206	21.117	1.00	29.87	C
	ATOM	388	C	LEU A 219	3.260	35.905	21.894	1.00	29.21	C
	ATOM	389	O	LEU A 219	2.710	34.869	21.516	1.00	29.73	O
5	ATOM	390	CB	LEU A 219	4.355	37.462	20.286	1.00	31.48	C
	ATOM	391	CG	LEU A 219	4.778	36.321	19.352	1.00	33.59	C
	ATOM	392	CD1	LEU A 219	3.700	36.083	18.301	1.00	34.93	C
	ATOM	393	CD2	LEU A 219	6.100	36.676	18.690	1.00	35.57	C
	ATOM	394	N	GLU A 220	4.018	35.963	22.982	1.00	28.82	N
10	ATOM	395	CA	GLU A 220	4.258	34.781	23.801	1.00	29.09	C
	ATOM	396	C	GLU A 220	2.958	34.194	24.342	1.00	29.07	C
	ATOM	397	O	GLU A 220	2.757	32.983	24.297	1.00	27.80	O
	ATOM	398	CB	GLU A 220	5.213	35.131	24.946	1.00	31.33	C
	ATOM	399	CG	GLU A 220	6.620	35.466	24.456	1.00	32.76	C
	ATOM	400	CD	GLU A 220	7.434	36.277	25.450	1.00	35.67	C
15	ATOM	401	OE1	GLU A 220	8.574	36.657	25.104	1.00	37.03	O
	ATOM	402	OE2	GLU A 220	6.944	36.541	26.569	1.00	36.27	O
	ATOM	403	N	LEU A 221	2.073	35.052	24.841	1.00	28.79	N
	ATOM	404	CA	LEU A 221	0.799	34.592	25.383	1.00	29.82	C
20	ATOM	405	C	LEU A 221	-0.143	34.089	24.293	1.00	29.77	C
	ATOM	406	O	LEU A 221	-0.923	33.165	24.516	1.00	30.04	O
	ATOM	407	CB	LEU A 221	0.125	35.714	26.181	1.00	30.05	C
	ATOM	408	CG	LEU A 221	0.743	36.046	27.544	1.00	31.65	C
	ATOM	409	CD1	LEU A 221	0.065	37.278	28.138	1.00	32.22	C
	ATOM	410	CD2	LEU A 221	0.588	34.850	28.482	1.00	31.89	C
25	ATOM	411	N	SER A 222	-0.066	34.687	23.108	1.00	31.28	N
	ATOM	412	CA	SER A 222	-0.931	34.272	22.011	1.00	32.25	C
	ATOM	413	C	SER A 222	-0.536	32.905	21.460	1.00	32.84	C
	ATOM	414	O	SER A 222	-1.380	32.170	20.947	1.00	33.76	O
30	ATOM	415	CB	SER A 222	-0.895	35.304	20.877	1.00	34.81	C
	ATOM	416	OG	SER A 222	0.367	35.315	20.230	1.00	39.03	O
	ATOM	417	N	GLN A 223	0.742	32.558	21.584	1.00	31.84	N
	ATOM	418	CA	GLN A 223	1.234	31.288	21.063	1.00	31.75	C
	ATOM	419	C	GLN A 223	1.596	30.215	22.089	1.00	30.53	C
35	ATOM	420	O	GLN A 223	1.306	29.039	21.869	1.00	30.69	O
	ATOM	421	CB	GLN A 223	2.434	31.550	20.151	1.00	34.71	C
	ATOM	422	CG	GLN A 223	2.066	32.296	18.873	1.00	38.65	C
	ATOM	423	CD	GLN A 223	3.275	32.719	18.065	1.00	42.46	C
	ATOM	424	OE1	GLN A 223	3.154	33.114	16.903	1.00	45.44	O
40	ATOM	425	NE2	GLN A 223	4.450	32.652	18.679	1.00	44.57	N
	ATOM	426	N	LEU A 224	2.226	30.610	23.195	1.00	28.64	N
	ATOM	427	CA	LEU A 224	2.632	29.654	24.232	1.00	27.07	C
	ATOM	428	C	LEU A 224	3.209	28.401	23.569	1.00	26.40	C
	ATOM	429	O	LEU A 224	2.898	27.274	23.962	1.00	25.81	O
45	ATOM	430	CB	LEU A 224	1.424	29.276	25.102	1.00	27.70	C
	ATOM	431	CG	LEU A 224	0.785	30.424	25.893	1.00	27.88	C
	ATOM	432	CD1	LEU A 224	-0.463	29.931	26.615	1.00	29.53	C
	ATOM	433	CD2	LEU A 224	1.789	30.981	26.884	1.00	27.54	C
	ATOM	434	N	SER A 225	4.071	28.614	22.577	1.00	25.74	N
50	ATOM	435	CA	SER A 225	4.667	27.531	21.798	1.00	25.83	C
	ATOM	436	C	SER A 225	5.454	26.473	22.563	1.00	25.18	C
	ATOM	437	O	SER A 225	5.446	25.302	22.182	1.00	25.89	O
	ATOM	438	CB	SER A 225	5.557	28.110	20.696	1.00	26.31	C
	ATOM	439	OG	SER A 225	6.710	28.731	21.233	1.00	29.36	O
55	ATOM	440	N	MET A 226	6.132	26.880	23.630	1.00	24.58	N
	ATOM	441	CA	MET A 226	6.931	25.948	24.424	1.00	24.51	C
	ATOM	442	C	MET A 226	6.193	25.387	25.631	1.00	24.00	C
	ATOM	443	O	MET A 226	6.725	24.529	26.336	1.00	24.19	O
	ATOM	444	CB	MET A 226	8.219	26.629	24.905	1.00	24.70	C

-138-

	ATOM	445	CG	MET	A	226	9.329	26.715	23.870	1.00	25.85	C
	ATOM	446	SD	MET	A	226	9.960	25.094	23.351	1.00	27.27	S
	ATOM	447	CE	MET	A	226	10.773	24.531	24.858	1.00	28.07	C
5	ATOM	448	N	LEU	A	227	4.969	25.850	25.872	1.00	23.05	N
	ATOM	449	CA	LEU	A	227	4.225	25.377	27.030	1.00	23.85	C
	ATOM	450	C	LEU	A	227	3.882	23.887	27.032	1.00	23.65	C
	ATOM	451	O	LEU	A	227	4.062	23.218	28.052	1.00	24.44	O
	ATOM	452	CB	LEU	A	227	2.949	26.212	27.237	1.00	24.02	C
10	ATOM	453	CG	LEU	A	227	2.139	25.868	28.494	1.00	24.67	C
	ATOM	454	CD1	LEU	A	227	3.019	25.994	29.730	1.00	25.75	C
	ATOM	455	CD2	LEU	A	227	0.936	26.798	28.612	1.00	25.81	C
	ATOM	456	N	PRO	A	228	3.395	23.336	25.901	1.00	24.00	N
	ATOM	457	CA	PRO	A	228	3.073	21.904	25.931	1.00	23.78	C
15	ATOM	458	C	PRO	A	228	4.261	21.024	26.330	1.00	23.69	C
	ATOM	459	O	PRO	A	228	4.123	20.109	27.155	1.00	23.20	O
	ATOM	460	CB	PRO	A	228	2.602	21.626	24.504	1.00	24.23	C
	ATOM	461	CG	PRO	A	228	1.957	22.939	24.110	1.00	24.58	C
	ATOM	462	CD	PRO	A	228	2.962	23.948	24.629	1.00	23.63	C
20	ATOM	463	N	HIS	A	229	5.421	21.305	25.747	1.00	22.38	N
	ATOM	464	CA	HIS	A	229	6.626	20.532	26.037	1.00	22.16	C
	ATOM	465	C	HIS	A	229	7.089	20.679	27.490	1.00	21.32	C
	ATOM	466	O	HIS	A	229	7.409	19.687	28.151	1.00	20.38	O
	ATOM	467	CB	HIS	A	229	7.765	20.951	25.103	1.00	22.65	C
25	ATOM	468	CG	HIS	A	229	9.037	20.196	25.337	1.00	23.54	C
	ATOM	469	ND1	HIS	A	229	9.235	18.910	24.883	1.00	24.88	N
	ATOM	470	CD2	HIS	A	229	10.160	20.535	26.012	1.00	23.99	C
	ATOM	471	CE1	HIS	A	229	10.427	18.488	25.270	1.00	25.42	C
	ATOM	472	NE2	HIS	A	229	11.009	19.455	25.957	1.00	23.32	N
30	ATOM	473	N	LEU	A	230	7.139	21.913	27.985	1.00	20.90	N
	ATOM	474	CA	LEU	A	230	7.578	22.139	29.355	1.00	21.22	C
	ATOM	475	C	LEU	A	230	6.563	21.623	30.361	1.00	21.08	C
	ATOM	476	O	LEU	A	230	6.938	21.164	31.435	1.00	19.50	O
	ATOM	477	CB	LEU	A	230	7.858	23.625	29.602	1.00	21.98	C
35	ATOM	478	CG	LEU	A	230	9.051	24.211	28.839	1.00	23.32	C
	ATOM	479	CD1	LEU	A	230	9.285	25.637	29.322	1.00	25.98	C
	ATOM	480	CD2	LEU	A	230	10.311	23.371	29.073	1.00	24.89	C
	ATOM	481	N	ALA	A	231	5.279	21.703	30.022	1.00	20.40	N
	ATOM	482	CA	ALA	A	231	4.243	21.197	30.917	1.00	21.50	C
40	ATOM	483	C	ALA	A	231	4.421	19.685	31.040	1.00	21.12	C
	ATOM	484	O	ALA	A	231	4.303	19.124	32.129	1.00	21.78	O
	ATOM	485	CB	ALA	A	231	2.859	21.522	30.361	1.00	22.95	C
	ATOM	486	N	ASP	A	232	4.707	19.028	29.919	1.00	20.87	N
	ATOM	487	CA	ASP	A	232	4.910	17.582	29.916	1.00	21.48	C
45	ATOM	488	C	ASP	A	232	6.168	17.228	30.711	1.00	20.43	C
	ATOM	489	O	ASP	A	232	6.167	16.259	31.463	1.00	21.59	O
	ATOM	490	CB	ASP	A	232	5.022	17.056	28.482	1.00	21.87	C
	ATOM	491	CG	ASP	A	232	3.664	16.893	27.807	1.00	25.14	C
	ATOM	492	OD1	ASP	A	232	3.639	16.665	26.582	1.00	26.65	O
50	ATOM	493	OD2	ASP	A	232	2.623	16.982	28.497	1.00	25.49	O
	ATOM	494	N	LEU	A	233	7.228	18.018	30.549	1.00	21.20	N
	ATOM	495	CA	LEU	A	233	8.483	17.785	31.278	1.00	20.50	C
	ATOM	496	C	LEU	A	233	8.267	17.940	32.785	1.00	20.58	C
	ATOM	497	O	LEU	A	233	8.755	17.139	33.587	1.00	18.39	O
55	ATOM	498	CB	LEU	A	233	9.565	18.770	30.811	1.00	20.92	C
	ATOM	499	CG	LEU	A	233	10.826	18.839	31.684	1.00	20.96	C
	ATOM	500	CD1	LEU	A	233	11.554	17.502	31.652	1.00	22.15	C
	ATOM	501	CD2	LEU	A	233	11.737	19.969	31.190	1.00	22.47	C
	ATOM	502	N	VAL	A	234	7.539	18.981	33.172	1.00	20.09	N

-139-

	ATOM	503	CA	VAL A 234	7.263	19.217	34.583	1.00	20.15	C
	ATOM	504	C	VAL A 234	6.320	18.152	35.146	1.00	19.97	C
	ATOM	505	O	VAL A 234	6.500	17.691	36.268	1.00	19.99	O
5	ATOM	506	CB	VAL A 234	6.665	20.630	34.796	1.00	21.02	C
	ATOM	507	CG1	VAL A 234	6.104	20.778	36.209	1.00	23.20	C
	ATOM	508	CG2	VAL A 234	7.754	21.679	34.566	1.00	21.83	C
	ATOM	509	N	SER A 235	5.324	17.749	34.362	1.00	18.23	N
	ATOM	510	CA	SER A 235	4.378	16.732	34.821	1.00	19.68	C
10	ATOM	511	C	SER A 235	5.117	15.413	35.079	1.00	19.46	C
	ATOM	512	O	SER A 235	4.906	14.743	36.095	1.00	19.95	O
	ATOM	513	CB	SER A 235	3.284	16.537	33.767	1.00	21.15	C
	ATOM	514	OG	SER A 235	2.229	15.734	34.274	1.00	26.38	O
	ATOM	515	N	TYR A 236	5.983	15.057	34.140	1.00	19.05	N
15	ATOM	516	CA	TYR A 236	6.796	13.849	34.222	1.00	19.13	C
	ATOM	517	C	TYR A 236	7.660	13.930	35.479	1.00	18.86	C
	ATOM	518	O	TYR A 236	7.792	12.958	36.223	1.00	18.39	O
	ATOM	519	CB	TYR A 236	7.675	13.781	32.976	1.00	19.07	C
	ATOM	520	CG	TYR A 236	8.800	12.764	32.990	1.00	19.18	C
20	ATOM	521	CD1	TYR A 236	8.601	11.466	32.527	1.00	20.38	C
	ATOM	522	CD2	TYR A 236	10.084	13.131	33.391	1.00	20.55	C
	ATOM	523	CE1	TYR A 236	9.665	10.557	32.448	1.00	21.48	C
	ATOM	524	CE2	TYR A 236	11.149	12.233	33.321	1.00	20.66	C
	ATOM	525	CZ	TYR A 236	10.934	10.954	32.846	1.00	21.96	C
	ATOM	526	OH	TYR A 236	11.996	10.079	32.749	1.00	21.78	O
25	ATOM	527	N	SER A 237	8.241	15.105	35.711	1.00	17.93	N
	ATOM	528	CA	SER A 237	9.106	15.312	36.868	1.00	18.19	C
	ATOM	529	C	SER A 237	8.373	15.218	38.199	1.00	18.73	C
	ATOM	530	O	SER A 237	8.929	14.737	39.184	1.00	19.34	O
30	ATOM	531	CB	SER A 237	9.830	16.654	36.730	1.00	18.72	C
	ATOM	532	OG	SER A 237	10.648	16.628	35.573	1.00	19.76	O
	ATOM	533	N	ILE A 238	7.128	15.680	38.237	1.00	18.89	N
	ATOM	534	CA	ILE A 238	6.343	15.597	39.460	1.00	20.25	C
	ATOM	535	C	ILE A 238	6.101	14.119	39.759	1.00	20.17	C
35	ATOM	536	O	ILE A 238	6.129	13.705	40.914	1.00	20.62	O
	ATOM	537	CB	ILE A 238	4.984	16.337	39.317	1.00	21.21	C
	ATOM	538	CG1	ILE A 238	5.226	17.847	39.236	1.00	23.61	C
	ATOM	539	CG2	ILE A 238	4.068	16.001	40.502	1.00	23.76	C
	ATOM	540	CD1	ILE A 238	3.972	18.668	38.937	1.00	24.70	C
40	ATOM	541	N	GLN A 239	5.868	13.315	38.719	1.00	20.04	N
	ATOM	542	CA	GLN A 239	5.657	11.890	38.936	1.00	19.72	C
	ATOM	543	C	GLN A 239	6.911	11.261	39.531	1.00	20.24	C
	ATOM	544	O	GLN A 239	6.823	10.433	40.437	1.00	19.92	O
	ATOM	545	CB	GLN A 239	5.288	11.178	37.628	1.00	21.35	C
45	ATOM	546	CG	GLN A 239	3.920	11.576	37.086	1.00	21.87	C
	ATOM	547	CD	GLN A 239	3.487	10.707	35.922	1.00	23.58	C
	ATOM	548	OE1	GLN A 239	3.092	9.556	36.105	1.00	26.39	O
	ATOM	549	NE2	GLN A 239	3.568	11.249	34.720	1.00	22.31	N
	ATOM	550	N	LYS A 240	8.080	11.661	39.037	1.00	19.37	N
50	ATOM	551	CA	LYS A 240	9.336	11.116	39.557	1.00	19.49	C
	ATOM	552	C	LYS A 240	9.575	11.583	40.994	1.00	20.03	C
	ATOM	553	O	LYS A 240	10.086	10.826	41.826	1.00	20.81	O
	ATOM	554	CB	LYS A 240	10.509	11.525	38.658	1.00	19.27	C
	ATOM	555	CG	LYS A 240	10.385	11.015	37.216	1.00	19.70	C
	ATOM	556	CD	LYS A 240	10.174	9.491	37.165	1.00	20.85	C
55	ATOM	557	CE	LYS A 240	10.201	8.986	35.734	1.00	20.78	C
	ATOM	558	NZ	LYS A 240	9.919	7.527	35.631	1.00	21.79	N
	ATOM	559	N	VAL A 241	9.203	12.827	41.284	1.00	19.95	N
	ATOM	560	CA	VAL A 241	9.355	13.380	42.630	1.00	21.18	C

-140-

	ATOM	561	C	VAL A 241	8.466	12.633	43.621	1.00	22.58	C
	ATOM	562	O	VAL A 241	8.845	12.418	44.769	1.00	22.01	O
	ATOM	563	CB	VAL A 241	9.006	14.890	42.658	1.00	22.53	C
5	ATOM	564	CG1	VAL A 241	8.893	15.392	44.104	1.00	23.49	C
	ATOM	565	CG2	VAL A 241	10.092	15.671	41.929	1.00	22.43	C
	ATOM	566	N	ILE A 242	7.277	12.237	43.178	1.00	22.44	N
	ATOM	567	CA	ILE A 242	6.375	11.492	44.052	1.00	23.64	C
	ATOM	568	C	ILE A 242	7.027	10.157	44.416	1.00	23.45	C
10	ATOM	569	O	ILE A 242	6.987	9.726	45.573	1.00	25.50	O
	ATOM	570	CB	ILE A 242	5.012	11.255	43.360	1.00	24.32	C
	ATOM	571	CG1	ILE A 242	4.235	12.575	43.303	1.00	25.64	C
	ATOM	572	CG2	ILE A 242	4.214	10.186	44.104	1.00	24.95	C
	ATOM	573	CD1	ILE A 242	3.012	12.540	42.401	1.00	25.41	C
15	ATOM	574	N	GLY A 243	7.652	9.521	43.431	1.00	22.76	N
	ATOM	575	CA	GLY A 243	8.310	8.246	43.665	1.00	23.14	C
	ATOM	576	C	GLY A 243	9.491	8.385	44.604	1.00	23.29	C
	ATOM	577	O	GLY A 243	9.719	7.525	45.454	1.00	24.26	O
	ATOM	578	N	PHE A 244	10.244	9.471	44.443	1.00	22.21	N
20	ATOM	579	CA	PHE A 244	11.406	9.754	45.287	1.00	23.08	C
	ATOM	580	C	PHE A 244	10.962	9.960	46.734	1.00	23.33	C
	ATOM	581	O	PHE A 244	11.509	9.359	47.665	1.00	22.96	O
	ATOM	582	CB	PHE A 244	12.110	11.023	44.799	1.00	21.55	C
	ATOM	583	CG	PHE A 244	13.264	11.454	45.663	1.00	23.20	C
25	ATOM	584	CD1	PHE A 244	14.474	10.764	45.632	1.00	25.04	C
	ATOM	585	CD2	PHE A 244	13.140	12.548	46.516	1.00	24.78	C
	ATOM	586	CE1	PHE A 244	15.542	11.157	46.437	1.00	25.46	C
	ATOM	587	CE2	PHE A 244	14.205	12.950	47.327	1.00	24.71	C
	ATOM	588	CZ	PHE A 244	15.407	12.254	47.286	1.00	24.22	C
30	ATOM	589	N	ALA A 245	9.963	10.819	46.912	1.00	23.25	N
	ATOM	590	CA	ALA A 245	9.441	11.134	48.233	1.00	23.37	C
	ATOM	591	C	ALA A 245	8.960	9.906	49.006	1.00	25.09	C
	ATOM	592	O	ALA A 245	9.182	9.805	50.212	1.00	24.87	O
	ATOM	593	CB	ALA A 245	8.310	12.156	48.113	1.00	22.36	C
35	ATOM	594	N	LYS A 246	8.309	8.975	48.314	1.00	26.15	N
	ATOM	595	CA	LYS A 246	7.800	7.768	48.959	1.00	28.66	C
	ATOM	596	C	LYS A 246	8.914	6.918	49.562	1.00	29.21	C
	ATOM	597	O	LYS A 246	8.668	6.117	50.466	1.00	29.75	O
	ATOM	598	CB	LYS A 246	6.997	6.931	47.957	1.00	30.93	C
40	ATOM	599	CG	LYS A 246	5.702	7.593	47.501	1.00	34.75	C
	ATOM	600	CD	LYS A 246	5.017	6.811	46.383	1.00	37.28	C
	ATOM	601	CE	LYS A 246	4.410	5.501	46.873	1.00	40.02	C
	ATOM	602	NZ	LYS A 246	3.230	5.724	47.756	1.00	42.15	N
	ATOM	603	N	MET A 247	10.138	7.104	49.074	1.00	28.68	N
45	ATOM	604	CA	MET A 247	11.282	6.339	49.562	1.00	29.45	C
	ATOM	605	C	MET A 247	12.076	7.021	50.681	1.00	28.75	C
	ATOM	606	O	MET A 247	13.012	6.431	51.230	1.00	28.61	O
	ATOM	607	CB	MET A 247	12.219	5.990	48.396	1.00	30.97	C
	ATOM	608	CG	MET A 247	11.614	5.007	47.393	1.00	34.76	C
50	ATOM	609	SD	MET A 247	12.766	4.475	46.096	1.00	39.72	S
	ATOM	610	CE	MET A 247	12.303	5.554	44.763	1.00	39.07	C
	ATOM	611	N	ILE A 248	11.709	8.253	51.023	1.00	27.31	N
	ATOM	612	CA	ILE A 248	12.391	8.973	52.100	1.00	28.07	C
	ATOM	613	C	ILE A 248	12.033	8.295	53.420	1.00	28.99	C
55	ATOM	614	O	ILE A 248	10.859	8.179	53.763	1.00	28.97	O
	ATOM	615	CB	ILE A 248	11.934	10.446	52.195	1.00	27.49	C
	ATOM	616	CG1	ILE A 248	12.299	11.198	50.916	1.00	26.51	C
	ATOM	617	CG2	ILE A 248	12.582	11.114	53.411	1.00	28.63	C
	ATOM	618	CD1	ILE A 248	11.730	12.605	50.865	1.00	25.47	C

-141-

	ATOM	619	N	PRO A 249	13.041	7.844	54.181	1.00	30.64	N
	ATOM	620	CA	PRO A 249	12.764	7.182	55.460	1.00	31.91	C
	ATOM	621	C	PRO A 249	11.818	7.992	56.348	1.00	32.16	C
5	ATOM	622	O	PRO A 249	12.107	9.138	56.688	1.00	34.02	O
	ATOM	623	CB	PRO A 249	14.153	7.035	56.075	1.00	32.36	C
	ATOM	624	CG	PRO A 249	15.021	6.835	54.871	1.00	32.23	C
	ATOM	625	CD	PRO A 249	14.490	7.890	53.917	1.00	30.61	C
	ATOM	626	N	GLY A 250	10.686	7.392	56.706	1.00	32.30	N
10	ATOM	627	CA	GLY A 250	9.725	8.064	57.565	1.00	33.31	C
	ATOM	628	C	GLY A 250	8.542	8.700	56.858	1.00	33.48	C
	ATOM	629	O	GLY A 250	7.484	8.888	57.459	1.00	33.45	O
	ATOM	630	N	PHE A 251	8.709	9.023	55.579	1.00	33.51	N
	ATOM	631	CA	PHE A 251	7.643	9.658	54.809	1.00	33.69	C
15	ATOM	632	C	PHE A 251	6.335	8.871	54.833	1.00	34.57	C
	ATOM	633	O	PHE A 251	5.259	9.455	54.964	1.00	35.10	O
	ATOM	634	CB	PHE A 251	8.082	9.850	53.356	1.00	31.35	C
	ATOM	635	CG	PHE A 251	7.180	10.754	52.564	1.00	29.89	C
	ATOM	636	CD1	PHE A 251	7.234	12.134	52.735	1.00	30.12	C
20	ATOM	637	CD2	PHE A 251	6.276	10.227	51.643	1.00	30.05	C
	ATOM	638	CE1	PHE A 251	6.400	12.979	51.999	1.00	29.28	C
	ATOM	639	CE2	PHE A 251	5.441	11.063	50.906	1.00	28.78	C
	ATOM	640	CZ	PHE A 251	5.505	12.440	51.085	1.00	28.48	C
	ATOM	641	N	ARG A 252	6.431	7.551	54.703	1.00	36.83	N
25	ATOM	642	CA	ARG A 252	5.250	6.691	54.698	1.00	39.19	C
	ATOM	643	C	ARG A 252	4.535	6.647	56.045	1.00	39.61	C
	ATOM	644	O	ARG A 252	3.391	6.200	56.127	1.00	40.31	O
	ATOM	645	CB	ARG A 252	5.625	5.262	54.292	1.00	41.06	C
	ATOM	646	CG	ARG A 252	6.138	5.101	52.867	1.00	44.96	C
30	ATOM	647	CD	ARG A 252	6.260	3.620	52.516	1.00	47.63	C
	ATOM	648	NE	ARG A 252	6.777	3.393	51.169	1.00	50.79	N
	ATOM	649	CZ	ARG A 252	8.062	3.459	50.831	1.00	51.79	C
	ATOM	650	NH1	ARG A 252	8.982	3.745	51.745	1.00	52.82	N
	ATOM	651	NH2	ARG A 252	8.427	3.235	49.576	1.00	52.64	N
35	ATOM	652	N	ASP A 253	5.205	7.102	57.098	1.00	39.96	N
	ATOM	653	CA	ASP A 253	4.610	7.097	58.430	1.00	40.45	C
	ATOM	654	C	ASP A 253	3.648	8.255	58.635	1.00	39.90	C
	ATOM	655	O	ASP A 253	2.902	8.284	59.612	1.00	39.68	O
	ATOM	656	CB	ASP A 253	5.698	7.127	59.506	1.00	42.53	C
40	ATOM	657	CG	ASP A 253	6.524	5.856	59.531	1.00	44.84	C
	ATOM	658	OD1	ASP A 253	5.938	4.767	59.345	1.00	47.60	O
	ATOM	659	OD2	ASP A 253	7.752	5.942	59.743	1.00	45.66	O
	ATOM	660	N	LEU A 254	3.669	9.208	57.710	1.00	38.00	N
	ATOM	661	CA	LEU A 254	2.782	10.361	57.780	1.00	37.81	C
45	ATOM	662	C	LEU A 254	1.417	9.978	57.218	1.00	37.76	C
	ATOM	663	O	LEU A 254	1.293	9.000	56.476	1.00	37.49	O
	ATOM	664	CB	LEU A 254	3.348	11.521	56.955	1.00	36.51	C
	ATOM	665	CG	LEU A 254	4.707	12.101	57.346	1.00	36.86	C
	ATOM	666	CD1	LEU A 254	5.142	13.113	56.297	1.00	35.66	C
50	ATOM	667	CD2	LEU A 254	4.620	12.751	58.719	1.00	36.85	C
	ATOM	668	N	THR A 255	0.395	10.745	57.579	1.00	38.14	N
	ATOM	669	CA	THR A 255	-0.950	10.496	57.077	1.00	39.08	C
	ATOM	670	C	THR A 255	-0.928	10.828	55.588	1.00	39.76	C
	ATOM	671	O	THR A 255	-0.075	11.593	55.139	1.00	39.15	O
55	ATOM	672	CB	THR A 255	-1.982	11.397	57.781	1.00	39.68	C
	ATOM	673	OG1	THR A 255	-1.573	12.767	57.677	1.00	39.47	O
	ATOM	674	CG2	THR A 255	-2.105	11.020	59.253	1.00	40.24	C
	ATOM	675	N	SER A 256	-1.851	10.258	54.817	1.00	40.24	N
	ATOM	676	CA	SER A 256	-1.883	10.527	53.382	1.00	40.92	C

-142-

	ATOM	677	C	SER A 256	-2.148	12.010	53.152	1.00	40.23	C
	ATOM	678	O	SER A 256	-1.662	12.599	52.185	1.00	40.28	O
	ATOM	679	CB	SER A 256	-2.968	9.693	52.690	1.00	41.53	C
5	ATOM	680	OG	SER A 256	-4.263	10.203	52.957	1.00	43.52	O
	ATOM	681	N	GLU A 257	-2.916	12.610	54.056	1.00	39.55	N
	ATOM	682	CA	GLU A 257	-3.252	14.024	53.963	1.00	38.71	C
	ATOM	683	C	GLU A 257	-1.999	14.889	54.038	1.00	36.50	C
	ATOM	684	O	GLU A 257	-1.825	15.810	53.240	1.00	36.20	O
10	ATOM	685	CB	GLU A 257	-4.221	14.400	55.085	1.00	41.43	C
	ATOM	686	CG	GLU A 257	-4.650	15.853	55.090	1.00	44.63	C
	ATOM	687	CD	GLU A 257	-5.747	16.121	56.103	1.00	47.39	C
	ATOM	688	OE1	GLU A 257	-6.879	15.634	55.896	1.00	48.76	O
	ATOM	689	OE2	GLU A 257	-5.476	16.810	57.109	1.00	48.99	O
	ATOM	690	N	ASP A 258	-1.132	14.593	55.001	1.00	34.59	N
15	ATOM	691	CA	ASP A 258	0.111	15.339	55.159	1.00	33.04	C
	ATOM	692	C	ASP A 258	1.064	15.047	54.002	1.00	32.48	C
	ATOM	693	O	ASP A 258	1.782	15.934	53.546	1.00	31.37	O
	ATOM	694	CB	ASP A 258	0.784	14.984	56.488	1.00	34.07	C
20	ATOM	695	CG	ASP A 258	0.256	15.809	57.645	1.00	35.11	C
	ATOM	696	OD1	ASP A 258	0.599	15.501	58.807	1.00	35.63	O
	ATOM	697	OD2	ASP A 258	-0.493	16.775	57.386	1.00	34.86	O
	ATOM	698	N	GLN A 259	1.072	13.803	53.532	1.00	31.90	N
	ATOM	699	CA	GLN A 259	1.940	13.433	52.417	1.00	32.81	C
	ATOM	700	C	GLN A 259	1.611	14.272	51.184	1.00	32.59	C
25	ATOM	701	O	GLN A 259	2.505	14.820	50.534	1.00	32.51	O
	ATOM	702	CB	GLN A 259	1.783	11.946	52.077	1.00	32.98	C
	ATOM	703	CG	GLN A 259	2.217	11.000	53.181	1.00	34.94	C
	ATOM	704	CD	GLN A 259	2.168	9.547	52.755	1.00	37.19	C
	ATOM	705	OE1	GLN A 259	2.322	8.641	53.576	1.00	39.55	O
30	ATOM	706	NE2	GLN A 259	1.958	9.315	51.466	1.00	37.81	N
	ATOM	707	N	ILE A 260	0.325	14.375	50.866	1.00	32.68	N
	ATOM	708	CA	ILE A 260	-0.109	15.147	49.706	1.00	32.42	C
	ATOM	709	C	ILE A 260	0.183	16.634	49.880	1.00	31.57	C
	ATOM	710	O	ILE A 260	0.588	17.311	48.933	1.00	30.43	O
35	ATOM	711	CB	ILE A 260	-1.619	14.959	49.445	1.00	33.97	C
	ATOM	712	CG1	ILE A 260	-1.933	13.471	49.277	1.00	34.59	C
	ATOM	713	CG2	ILE A 260	-2.036	15.731	48.201	1.00	33.83	C
	ATOM	714	CD1	ILE A 260	-1.156	12.789	48.165	1.00	36.85	C
	ATOM	715	N	VAL A 261	-0.029	17.146	51.088	1.00	29.87	N
40	ATOM	716	CA	VAL A 261	0.244	18.551	51.358	1.00	28.91	C
	ATOM	717	C	VAL A 261	1.717	18.862	51.097	1.00	27.91	C
	ATOM	718	O	VAL A 261	2.043	19.856	50.445	1.00	28.13	O
	ATOM	719	CB	VAL A 261	-0.089	18.923	52.827	1.00	28.91	C
	ATOM	720	CG1	VAL A 261	0.472	20.294	53.161	1.00	30.09	C
45	ATOM	721	CG2	VAL A 261	-1.594	18.911	53.035	1.00	31.46	C
	ATOM	722	N	LEU A 262	2.605	18.011	51.604	1.00	27.17	N
	ATOM	723	CA	LEU A 262	4.039	18.222	51.423	1.00	25.81	C
	ATOM	724	C	LEU A 262	4.461	18.126	49.955	1.00	25.46	C
	ATOM	725	O	LEU A 262	5.274	18.921	49.485	1.00	24.78	O
50	ATOM	726	CB	LEU A 262	4.836	17.219	52.265	1.00	26.02	C
	ATOM	727	CG	LEU A 262	4.604	17.278	53.781	1.00	25.71	C
	ATOM	728	CD1	LEU A 262	5.382	16.162	54.464	1.00	26.98	C
	ATOM	729	CD2	LEU A 262	5.028	18.634	54.317	1.00	26.30	C
	ATOM	730	N	LEU A 263	3.911	17.155	49.232	1.00	25.71	N
55	ATOM	731	CA	LEU A 263	4.244	16.985	47.818	1.00	26.15	C
	ATOM	732	C	LEU A 263	3.763	18.166	46.974	1.00	26.42	C
	ATOM	733	O	LEU A 263	4.514	18.702	46.154	1.00	25.91	O
	ATOM	734	CB	LEU A 263	3.633	15.681	47.283	1.00	27.20	C

-143-

	ATOM	735	CG	LEU	A	263	4.293	14.376	47.745	1.00	29.34	C
	ATOM	736	CD1	LEU	A	263	3.401	13.197	47.404	1.00	30.14	C
	ATOM	737	CD2	LEU	A	263	5.658	14.223	47.082	1.00	31.00	C
5	ATOM	738	N	LYS	A	264	2.519	18.585	47.178	1.00	25.69	N
	ATOM	739	CA	LYS	A	264	1.987	19.699	46.405	1.00	26.59	C
	ATOM	740	C	LYS	A	264	2.709	21.011	46.655	1.00	26.97	C
	ATOM	741	O	LYS	A	264	2.962	21.767	45.723	1.00	27.99	O
	ATOM	742	CB	LYS	A	264	0.496	19.899	46.688	1.00	29.36	C
10	ATOM	743	CG	LYS	A	264	-0.417	18.910	45.994	1.00	31.84	C
	ATOM	744	CD	LYS	A	264	-1.862	19.348	46.156	1.00	35.05	C
	ATOM	745	CE	LYS	A	264	-2.822	18.400	45.468	1.00	37.95	C
	ATOM	746	NZ	LYS	A	264	-4.233	18.872	45.629	1.00	39.41	N
	ATOM	747	N	SER	A	265	3.047	21.286	47.908	1.00	26.64	N
15	ATOM	748	CA	SER	A	265	3.712	22.540	48.227	1.00	27.75	C
	ATOM	749	C	SER	A	265	5.199	22.591	47.884	1.00	26.92	C
	ATOM	750	O	SER	A	265	5.750	23.676	47.723	1.00	28.28	O
	ATOM	751	CB	SER	A	265	3.513	22.881	49.709	1.00	28.81	C
	ATOM	752	OG	SER	A	265	4.101	21.902	50.540	1.00	33.64	O
20	ATOM	753	N	SER	A	266	5.847	21.434	47.757	1.00	25.17	N
	ATOM	754	CA	SER	A	266	7.277	21.412	47.449	1.00	23.91	C
	ATOM	755	C	SER	A	266	7.609	21.035	46.011	1.00	23.51	C
	ATOM	756	O	SER	A	266	8.749	21.206	45.572	1.00	23.30	O
	ATOM	757	CB	SER	A	266	8.001	20.445	48.385	1.00	24.45	C
25	ATOM	758	OG	SER	A	266	7.656	19.101	48.094	1.00	24.60	O
	ATOM	759	N	ALA	A	267	6.619	20.519	45.285	1.00	22.67	N
	ATOM	760	CA	ALA	A	267	6.801	20.089	43.898	1.00	23.39	C
	ATOM	761	C	ALA	A	267	7.698	20.979	43.040	1.00	23.51	C
	ATOM	762	O	ALA	A	267	8.716	20.517	42.515	1.00	23.55	O
30	ATOM	763	CB	ALA	A	267	5.436	19.938	43.217	1.00	24.51	C
	ATOM	764	N	ILE	A	268	7.330	22.247	42.883	1.00	22.01	N
	ATOM	765	CA	ILE	A	268	8.132	23.135	42.041	1.00	22.23	C
	ATOM	766	C	ILE	A	268	9.539	23.374	42.592	1.00	22.05	C
	ATOM	767	O	ILE	A	268	10.494	23.558	41.828	1.00	20.90	O
35	ATOM	768	CB	ILE	A	268	7.426	24.496	41.811	1.00	23.63	C
	ATOM	769	CG1	ILE	A	268	8.097	25.232	40.645	1.00	24.85	C
	ATOM	770	CG2	ILE	A	268	7.484	25.354	43.068	1.00	25.18	C
	ATOM	771	CD1	ILE	A	268	7.933	24.549	39.303	1.00	25.69	C
	ATOM	772	N	GLU	A	269	9.674	23.352	43.911	1.00	20.40	N
40	ATOM	773	CA	GLU	A	269	10.979	23.561	44.529	1.00	20.63	C
	ATOM	774	C	GLU	A	269	11.933	22.402	44.268	1.00	21.33	C
	ATOM	775	O	GLU	A	269	13.109	22.620	43.976	1.00	20.99	O
	ATOM	776	CB	GLU	A	269	10.823	23.770	46.030	1.00	20.38	C
	ATOM	777	CG	GLU	A	269	10.206	25.110	46.396	1.00	22.10	C
45	ATOM	778	CD	GLU	A	269	10.009	25.261	47.892	1.00	23.72	C
	ATOM	779	OE1	GLU	A	269	10.803	24.670	48.656	1.00	22.73	O
	ATOM	780	OE2	GLU	A	269	9.067	25.974	48.301	1.00	24.58	O
	ATOM	781	N	VAL	A	270	11.434	21.172	44.375	1.00	20.39	N
	ATOM	782	CA	VAL	A	270	12.279	20.006	44.143	1.00	20.83	C
50	ATOM	783	C	VAL	A	270	12.644	19.911	42.670	1.00	20.52	C
	ATOM	784	O	VAL	A	270	13.734	19.458	42.318	1.00	20.87	O
	ATOM	785	CB	VAL	A	270	11.582	18.709	44.597	1.00	21.55	C
	ATOM	786	CG1	VAL	A	270	12.481	17.512	44.318	1.00	21.95	C
	ATOM	787	CG2	VAL	A	270	11.268	18.790	46.086	1.00	23.25	C
55	ATOM	788	N	ILE	A	271	11.731	20.337	41.804	1.00	20.29	N
	ATOM	789	CA	ILE	A	271	12.010	20.318	40.376	1.00	20.71	C
	ATOM	790	C	ILE	A	271	13.145	21.300	40.099	1.00	20.86	C
	ATOM	791	O	ILE	A	271	14.083	20.990	39.361	1.00	20.78	O
	ATOM	792	CB	ILE	A	271	10.755	20.684	39.563	1.00	21.89	C

-144-

	ATOM	793	CG1	ILE	A	271	9.842	19.450	39.483	1.00	24.21	C
	ATOM	794	CG2	ILE	A	271	11.149	21.173	38.170	1.00	23.03	C
	ATOM	795	CD1	ILE	A	271	8.489	19.711	38.852	1.00	27.85	C
5	ATOM	796	N	MET	A	272	13.076	22.481	40.701	1.00	21.17	N
	ATOM	797	CA	MET	A	272	14.147	23.446	40.500	1.00	21.57	C
	ATOM	798	C	MET	A	272	15.474	22.888	41.020	1.00	20.82	C
	ATOM	799	O	MET	A	272	16.513	23.064	40.384	1.00	22.20	O
	ATOM	800	CB	MET	A	272	13.800	24.770	41.183	1.00	22.31	C
10	ATOM	801	CG	MET	A	272	12.595	25.441	40.549	1.00	24.16	C
	ATOM	802	SD	MET	A	272	12.222	27.036	41.296	1.00	26.22	S
	ATOM	803	CE	MET	A	272	11.003	27.687	40.134	1.00	26.38	C
	ATOM	804	N	LEU	A	273	15.442	22.204	42.163	1.00	21.17	N
	ATOM	805	CA	LEU	A	273	16.661	21.606	42.717	1.00	21.28	C
15	ATOM	806	C	LEU	A	273	17.226	20.486	41.842	1.00	20.96	C
	ATOM	807	O	LEU	A	273	18.408	20.494	41.487	1.00	20.75	O
	ATOM	808	CB	LEU	A	273	16.405	21.026	44.116	1.00	22.98	C
	ATOM	809	CG	LEU	A	273	16.367	21.940	45.337	1.00	25.62	C
	ATOM	810	CD1	LEU	A	273	15.959	21.129	46.572	1.00	25.83	C
20	ATOM	811	CD2	LEU	A	273	17.736	22.571	45.543	1.00	26.65	C
	ATOM	812	N	ARG	A	274	16.385	19.517	41.494	1.00	19.69	N
	ATOM	813	CA	ARG	A	274	16.852	18.384	40.702	1.00	19.52	C
	ATOM	814	C	ARG	A	274	17.317	18.787	39.309	1.00	19.10	C
	ATOM	815	O	ARG	A	274	18.159	18.117	38.715	1.00	19.83	O
25	ATOM	816	CB	ARG	A	274	15.759	17.299	40.610	1.00	19.75	C
	ATOM	817	CG	ARG	A	274	14.652	17.566	39.601	1.00	19.52	C
	ATOM	818	CD	ARG	A	274	13.381	16.792	39.969	1.00	19.72	C
	ATOM	819	NE	ARG	A	274	13.599	15.356	40.153	1.00	18.11	N
	ATOM	820	CZ	ARG	A	274	13.580	14.453	39.175	1.00	19.01	C
30	ATOM	821	NH1	ARG	A	274	13.357	14.824	37.919	1.00	18.53	N
	ATOM	822	NH2	ARG	A	274	13.759	13.168	39.458	1.00	19.51	N
	ATOM	823	N	SER	A	275	16.792	19.892	38.793	1.00	19.73	N
	ATOM	824	CA	SER	A	275	17.183	20.331	37.463	1.00	19.93	C
	ATOM	825	C	SER	A	275	18.615	20.838	37.442	1.00	19.90	C
35	ATOM	826	O	SER	A	275	19.191	21.016	36.377	1.00	20.21	O
	ATOM	827	CB	SER	A	275	16.249	21.437	36.958	1.00	20.51	C
	ATOM	828	OG	SER	A	275	16.520	22.680	37.579	1.00	20.38	O
	ATOM	829	N	ASN	A	276	19.198	21.055	38.615	1.00	20.28	N
	ATOM	830	CA	ASN	A	276	20.564	21.557	38.662	1.00	19.85	C
40	ATOM	831	C	ASN	A	276	21.512	20.544	38.024	1.00	21.26	C
	ATOM	832	O	ASN	A	276	22.585	20.903	37.538	1.00	19.72	O
	ATOM	833	CB	ASN	A	276	20.983	21.843	40.108	1.00	20.77	C
	ATOM	834	CG	ASN	A	276	22.265	22.651	40.187	1.00	23.39	C
	ATOM	835	OD1	ASN	A	276	23.275	22.187	40.713	1.00	26.18	O
45	ATOM	836	ND2	ASN	A	276	22.231	23.867	39.649	1.00	21.92	N
	ATOM	837	N	GLU	A	277	21.096	19.280	38.000	1.00	20.52	N
	ATOM	838	CA	GLU	A	277	21.925	18.226	37.425	1.00	21.75	C
	ATOM	839	C	GLU	A	277	22.103	18.370	35.908	1.00	21.79	C
	ATOM	840	O	GLU	A	277	23.105	17.910	35.351	1.00	22.41	O
50	ATOM	841	CB	GLU	A	277	21.331	16.852	37.785	1.00	22.91	C
	ATOM	842	CG	GLU	A	277	22.199	15.659	37.413	1.00	26.24	C
	ATOM	843	CD	GLU	A	277	21.904	14.418	38.261	1.00	28.07	C
	ATOM	844	OE1	GLU	A	277	22.359	13.319	37.875	1.00	30.43	O
	ATOM	845	OE2	GLU	A	277	21.233	14.532	39.317	1.00	26.56	O
55	ATOM	846	N	SER	A	278	21.152	19.011	35.234	1.00	19.68	N
	ATOM	847	CA	SER	A	278	21.266	19.194	33.789	1.00	20.64	C
	ATOM	848	C	SER	A	278	21.712	20.607	33.448	1.00	21.58	C
	ATOM	849	O	SER	A	278	22.008	20.910	32.292	1.00	22.05	O
	ATOM	850	CB	SER	A	278	19.934	18.910	33.092	1.00	20.93	C

-145-

	ATOM	851	OG	SER A 278	18.941	19.829	33.497	1.00	22.00	O
	ATOM	852	N	PHE A 279	21.751	21.474	34.451	1.00	21.92	N
	ATOM	853	CA	PHE A 279	22.160	22.853	34.219	1.00	23.24	C
5	ATOM	854	C	PHE A 279	23.659	22.912	33.972	1.00	24.55	C
	ATOM	855	O	PHE A 279	24.429	22.218	34.638	1.00	24.49	O
	ATOM	856	CB	PHE A 279	21.820	23.723	35.429	1.00	23.08	C
	ATOM	857	CG	PHE A 279	22.051	25.187	35.198	1.00	24.02	C
	ATOM	858	CD1	PHE A 279	21.135	25.942	34.471	1.00	24.96	C
10	ATOM	859	CD2	PHE A 279	23.197	25.805	35.682	1.00	24.94	C
	ATOM	860	CE1	PHE A 279	21.356	27.293	34.227	1.00	24.93	C
	ATOM	861	CE2	PHE A 279	23.429	27.160	35.442	1.00	25.50	C
	ATOM	862	CZ	PHE A 279	22.506	27.903	34.714	1.00	24.47	C
	ATOM	863	N	THR A 280	24.077	23.728	33.010	1.00	24.73	N
15	ATOM	864	CA	THR A 280	25.496	23.872	32.728	1.00	26.87	C
	ATOM	865	C	THR A 280	25.884	25.343	32.672	1.00	27.44	C
	ATOM	866	O	THR A 280	25.186	26.162	32.070	1.00	26.28	O
	ATOM	867	CB	THR A 280	25.897	23.198	31.399	1.00	27.76	C
	ATOM	868	OG1	THR A 280	27.298	23.408	31.173	1.00	31.72	O
20	ATOM	869	CG2	THR A 280	25.107	23.768	30.236	1.00	27.79	C
	ATOM	870	N	MET A 281	26.991	25.676	33.326	1.00	28.33	N
	ATOM	871	CA	MET A 281	27.469	27.049	33.340	1.00	31.03	C
	ATOM	872	C	MET A 281	28.275	27.390	32.095	1.00	31.28	C
	ATOM	873	O	MET A 281	28.812	28.490	31.980	1.00	30.87	O
25	ATOM	874	CB	MET A 281	28.298	27.306	34.596	1.00	33.43	C
	ATOM	875	CG	MET A 281	27.448	27.518	35.835	1.00	36.11	C
	ATOM	876	SD	MET A 281	28.429	27.829	37.295	1.00	39.85	S
	ATOM	877	CE	MET A 281	28.995	29.495	36.967	1.00	40.40	C
	ATOM	878	N	ASP A 282	28.364	26.448	31.159	1.00	31.72	N
30	ATOM	879	CA	ASP A 282	29.097	26.709	29.925	1.00	32.91	C
	ATOM	880	C	ASP A 282	28.366	27.818	29.175	1.00	32.02	C
	ATOM	881	O	ASP A 282	28.989	28.764	28.683	1.00	31.15	O
	ATOM	882	CB	ASP A 282	29.172	25.455	29.050	1.00	35.93	C
	ATOM	883	CG	ASP A 282	29.947	24.328	29.708	1.00	39.91	C
35	ATOM	884	OD1	ASP A 282	30.940	24.619	30.412	1.00	42.35	O
	ATOM	885	OD2	ASP A 282	29.573	23.150	29.508	1.00	42.45	O
	ATOM	886	N	ASP A 283	27.041	27.702	29.100	1.00	29.87	N
	ATOM	887	CA	ASP A 283	26.224	28.704	28.418	1.00	28.59	C
	ATOM	888	C	ASP A 283	24.931	29.032	29.170	1.00	27.92	C
40	ATOM	889	O	ASP A 283	23.984	29.568	28.592	1.00	27.21	O
	ATOM	890	CB	ASP A 283	25.904	28.243	26.994	1.00	29.84	C
	ATOM	891	CG	ASP A 283	25.030	27.006	26.958	1.00	31.11	C
	ATOM	892	OD1	ASP A 283	24.872	26.351	28.009	1.00	28.99	O
	ATOM	893	OD2	ASP A 283	24.507	26.687	25.870	1.00	32.79	O
45	ATOM	894	N	MET A 284	24.902	28.708	30.460	1.00	26.84	N
	ATOM	895	CA	MET A 284	23.748	28.985	31.317	1.00	27.62	C
	ATOM	896	C	MET A 284	22.449	28.379	30.801	1.00	27.20	C
	ATOM	897	O	MET A 284	21.429	29.060	30.686	1.00	27.86	O
	ATOM	898	CB	MET A 284	23.565	30.497	31.484	1.00	29.95	C
50	ATOM	899	CG	MET A 284	24.785	31.219	32.031	1.00	33.34	C
	ATOM	900	SD	MET A 284	25.323	30.578	33.624	1.00	36.23	S
	ATOM	901	CE	MET A 284	26.985	31.242	33.719	1.00	35.78	C
	ATOM	902	N	SER A 285	22.479	27.091	30.503	1.00	25.58	N
	ATOM	903	CA	SER A 285	21.288	26.427	30.010	1.00	24.62	C
55	ATOM	904	C	SER A 285	21.136	25.090	30.697	1.00	24.72	C
	ATOM	905	O	SER A 285	22.028	24.641	31.415	1.00	24.18	O
	ATOM	906	CB	SER A 285	21.402	26.186	28.509	1.00	24.98	C
	ATOM	907	OG	SER A 285	22.415	25.224	28.241	1.00	25.94	O
	ATOM	908	N	TRP A 286	19.982	24.472	30.480	1.00	24.17	N

-146-

	ATOM	909	CA	TRP	A	286	19.699	23.146	30.997	1.00	24.74	C
	ATOM	910	C	TRP	A	286	19.842	22.312	29.732	1.00	25.34	C
	ATOM	911	O	TRP	A	286	19.006	22.391	28.828	1.00	25.37	O
5	ATOM	912	CB	TRP	A	286	18.268	23.064	31.522	1.00	23.76	C
	ATOM	913	CG	TRP	A	286	18.048	23.702	32.863	1.00	21.76	C
	ATOM	914	CD1	TRP	A	286	18.186	23.107	34.088	1.00	21.47	C
	ATOM	915	CD2	TRP	A	286	17.568	25.031	33.118	1.00	23.03	C
	ATOM	916	NE1	TRP	A	286	17.811	23.976	35.084	1.00	21.88	N
10	ATOM	917	CE2	TRP	A	286	17.429	25.164	34.519	1.00	22.96	C
	ATOM	918	CE3	TRP	A	286	17.238	26.121	32.299	1.00	23.54	C
	ATOM	919	CZ2	TRP	A	286	16.970	26.341	35.120	1.00	24.15	C
	ATOM	920	CZ3	TRP	A	286	16.781	27.293	32.898	1.00	22.92	C
	ATOM	921	CH2	TRP	A	286	16.651	27.390	34.297	1.00	23.66	C
15	ATOM	922	N	THR	A	287	20.918	21.540	29.654	1.00	25.53	N
	ATOM	923	CA	THR	A	287	21.173	20.721	28.478	1.00	27.14	C
	ATOM	924	C	THR	A	287	20.833	19.266	28.753	1.00	27.53	C
	ATOM	925	O	THR	A	287	21.501	18.607	29.551	1.00	27.40	O
	ATOM	926	CB	THR	A	287	22.644	20.853	28.049	1.00	27.77	C
20	ATOM	927	OG1	THR	A	287	22.914	22.229	27.733	1.00	30.32	O
	ATOM	928	CG2	THR	A	287	22.922	20.000	26.824	1.00	29.69	C
	ATOM	929	N	CYS	A	288	19.792	18.775	28.084	1.00	28.08	N
	ATOM	930	CA	CYS	A	288	19.326	17.406	28.270	1.00	30.34	C
	ATOM	931	C	CYS	A	288	19.478	16.520	27.040	1.00	33.66	C
25	ATOM	932	O	CYS	A	288	18.530	15.857	26.624	1.00	33.19	O
	ATOM	933	CB	CYS	A	288	17.861	17.426	28.699	1.00	29.32	C
	ATOM	934	SG	CYS	A	288	17.566	18.403	30.188	1.00	28.01	S
	ATOM	935	N	GLY	A	289	20.675	16.498	26.466	1.00	37.69	N
	ATOM	936	CA	GLY	A	289	20.897	15.682	25.286	1.00	41.85	C
30	ATOM	937	C	GLY	A	289	21.072	16.536	24.044	1.00	44.11	C
	ATOM	938	O	GLY	A	289	21.842	17.497	24.051	1.00	45.10	O
	ATOM	939	N	ASN	A	290	20.349	16.205	22.978	1.00	46.33	N
	ATOM	940	CA	ASN	A	290	20.469	16.959	21.737	1.00	47.32	C
	ATOM	941	C	ASN	A	290	19.961	18.391	21.874	1.00	47.22	C
35	ATOM	942	O	ASN	A	290	19.303	18.746	22.857	1.00	47.49	O
	ATOM	943	CB	ASN	A	290	19.733	16.241	20.600	1.00	49.56	C
	ATOM	944	CG	ASN	A	290	18.235	16.224	20.792	1.00	51.07	C
	ATOM	945	OD1	ASN	A	290	17.591	17.271	20.803	1.00	52.29	O
	ATOM	946	ND2	ASN	A	290	17.668	15.032	20.944	1.00	51.45	N
40	ATOM	947	N	GLN	A	291	20.277	19.205	20.874	1.00	46.24	N
	ATOM	948	CA	GLN	A	291	19.896	20.611	20.850	1.00	45.60	C
	ATOM	949	C	GLN	A	291	18.402	20.859	21.031	1.00	43.20	C
	ATOM	950	O	GLN	A	291	18.007	21.916	21.520	1.00	43.27	O
	ATOM	951	CB	GLN	A	291	20.380	21.247	19.545	1.00	47.46	C
45	ATOM	952	CG	GLN	A	291	21.879	21.087	19.325	1.00	50.94	C
	ATOM	953	CD	GLN	A	291	22.705	21.786	20.395	1.00	52.59	C
	ATOM	954	OE1	GLN	A	291	23.893	21.503	20.563	1.00	54.12	O
	ATOM	955	NE2	GLN	A	291	22.081	22.712	21.114	1.00	53.69	N
	ATOM	956	N	ASP	A	292	17.574	19.897	20.636	1.00	40.92	N
50	ATOM	957	CA	ASP	A	292	16.129	20.046	20.780	1.00	38.58	C
	ATOM	958	C	ASP	A	292	15.740	20.140	22.252	1.00	35.80	C
	ATOM	959	O	ASP	A	292	14.769	20.814	22.601	1.00	34.04	O
	ATOM	960	CB	ASP	A	292	15.391	18.862	20.145	1.00	41.69	C
	ATOM	961	CG	ASP	A	292	15.325	18.950	18.629	1.00	44.13	C
55	ATOM	962	OD1	ASP	A	292	14.862	17.973	18.002	1.00	45.48	O
	ATOM	963	OD2	ASP	A	292	15.724	19.993	18.067	1.00	45.78	O
	ATOM	964	N	TYR	A	293	16.506	19.469	23.111	1.00	33.09	N
	ATOM	965	CA	TYR	A	293	16.219	19.465	24.543	1.00	31.43	C
	ATOM	966	C	TYR	A	293	17.183	20.305	25.367	1.00	30.28	C

-147-

	ATOM	967	O	TYR A 293	17.558	19.934	26.481	1.00	30.56	O
	ATOM	968	CB	TYR A 293	16.186	18.027	25.066	1.00	31.64	C
	ATOM	969	CG	TYR A 293	15.232	17.154	24.287	1.00	31.43	C
5	ATOM	970	CD1	TYR A 293	15.591	15.864	23.905	1.00	32.22	C
	ATOM	971	CD2	TYR A 293	13.999	17.647	23.861	1.00	32.09	C
	ATOM	972	CE1	TYR A 293	14.752	15.091	23.106	1.00	32.84	C
	ATOM	973	CE2	TYR A 293	13.153	16.883	23.063	1.00	31.78	C
	ATOM	974	CZ	TYR A 293	13.537	15.611	22.684	1.00	33.14	C
10	ATOM	975	OH	TYR A 293	12.726	14.874	21.850	1.00	32.75	O
	ATOM	976	N	LYS A 294	17.594	21.431	24.801	1.00	29.44	N
	ATOM	977	CA	LYS A 294	18.466	22.369	25.494	1.00	27.92	C
	ATOM	978	C	LYS A 294	17.529	23.530	25.786	1.00	27.57	C
	ATOM	979	O	LYS A 294	16.947	24.114	24.866	1.00	27.85	O
15	ATOM	980	CB	LYS A 294	19.618	22.833	24.595	1.00	31.41	C
	ATOM	981	CG	LYS A 294	20.500	23.907	25.239	1.00	32.77	C
	ATOM	982	CD	LYS A 294	21.578	24.416	24.284	1.00	36.06	C
	ATOM	983	CE	LYS A 294	22.872	23.633	24.419	1.00	37.32	C
	ATOM	984	NZ	LYS A 294	23.599	23.990	25.673	1.00	37.49	N
20	ATOM	985	N	TYR A 295	17.363	23.852	27.061	1.00	25.07	N
	ATOM	986	CA	TYR A 295	16.465	24.928	27.451	1.00	24.97	C
	ATOM	987	C	TYR A 295	17.208	26.154	27.938	1.00	25.69	C
	ATOM	988	O	TYR A 295	18.005	26.074	28.865	1.00	24.37	O
	ATOM	989	CB	TYR A 295	15.517	24.431	28.543	1.00	24.19	C
25	ATOM	990	CG	TYR A 295	14.927	23.080	28.216	1.00	24.03	C
	ATOM	991	CD1	TYR A 295	15.297	21.943	28.932	1.00	23.33	C
	ATOM	992	CD2	TYR A 295	14.023	22.933	27.167	1.00	23.84	C
	ATOM	993	CE1	TYR A 295	14.780	20.692	28.611	1.00	24.85	C
	ATOM	994	CE2	TYR A 295	13.500	21.688	26.836	1.00	24.18	C
30	ATOM	995	CZ	TYR A 295	13.882	20.573	27.563	1.00	24.74	C
	ATOM	996	OH	TYR A 295	13.369	19.338	27.244	1.00	24.72	O
	ATOM	997	N	ARG A 296	16.921	27.286	27.302	1.00	27.37	N
	ATOM	998	CA	ARG A 296	17.532	28.566	27.632	1.00	29.21	C
	ATOM	999	C	ARG A 296	16.457	29.505	28.177	1.00	28.74	C
35	ATOM	1000	O	ARG A 296	15.269	29.177	28.171	1.00	28.04	O
	ATOM	1001	CB	ARG A 296	18.140	29.201	26.377	1.00	31.67	C
	ATOM	1002	CG	ARG A 296	19.115	28.332	25.590	1.00	36.71	C
	ATOM	1003	CD	ARG A 296	19.581	29.091	24.352	1.00	40.42	C
	ATOM	1004	NE	ARG A 296	20.676	28.444	23.631	1.00	44.23	N
40	ATOM	1005	CZ	ARG A 296	20.533	27.442	22.769	1.00	46.02	C
	ATOM	1006	NH1	ARG A 296	19.329	26.949	22.508	1.00	46.77	N
	ATOM	1007	NH2	ARG A 296	21.597	26.941	22.152	1.00	46.52	N
	ATOM	1008	N	VAL A 297	16.879	30.678	28.634	1.00	29.11	N
	ATOM	1009	CA	VAL A 297	15.956	31.675	29.167	1.00	30.41	C
45	ATOM	1010	C	VAL A 297	14.821	31.972	28.187	1.00	30.24	C
	ATOM	1011	O	VAL A 297	13.655	32.065	28.582	1.00	29.94	O
	ATOM	1012	CB	VAL A 297	16.692	33.005	29.475	1.00	30.71	C
	ATOM	1013	CG1	VAL A 297	15.686	34.103	29.797	1.00	33.35	C
	ATOM	1014	CG2	VAL A 297	17.646	32.811	30.644	1.00	32.09	C
50	ATOM	1015	N	SER A 298	15.168	32.115	26.912	1.00	30.44	N
	ATOM	1016	CA	SER A 298	14.185	32.430	25.881	1.00	30.65	C
	ATOM	1017	C	SER A 298	13.106	31.370	25.714	1.00	30.99	C
	ATOM	1018	O	SER A 298	11.986	31.680	25.304	1.00	31.34	O
	ATOM	1019	CB	SER A 298	14.884	32.675	24.539	1.00	31.86	C
55	ATOM	1020	OG	SER A 298	15.658	31.559	24.143	1.00	33.35	O
	ATOM	1021	N	ASP A 299	13.435	30.121	26.028	1.00	29.88	N
	ATOM	1022	CA	ASP A 299	12.464	29.042	25.912	1.00	29.41	C
	ATOM	1023	C	ASP A 299	11.424	29.137	27.019	1.00	28.20	C
	ATOM	1024	O	ASP A 299	10.268	28.770	26.827	1.00	28.75	O

-148-

	ATOM	1025	CB	ASP	A	299	13.162	27.679	25.979	1.00	31.09	C
	ATOM	1026	CG	ASP	A	299	14.070	27.435	24.797	1.00	34.22	C
	ATOM	1027	OD1	ASP	A	299	13.589	27.548	23.651	1.00	34.74	O
	ATOM	1028	OD2	ASP	A	299	15.263	27.129	25.013	1.00	36.25	O
5	ATOM	1029	N	VAL	A	300	11.837	29.631	28.183	1.00	27.61	N
	ATOM	1030	CA	VAL	A	300	10.923	29.760	29.308	1.00	26.53	C
	ATOM	1031	C	VAL	A	300	9.948	30.913	29.070	1.00	26.97	C
	ATOM	1032	O	VAL	A	300	8.781	30.835	29.449	1.00	26.32	O
	ATOM	1033	CB	VAL	A	300	11.703	29.972	30.623	1.00	27.74	C
10	ATOM	1034	CG1	VAL	A	300	10.749	29.958	31.811	1.00	29.57	C
	ATOM	1035	CG2	VAL	A	300	12.757	28.871	30.772	1.00	27.69	C
	ATOM	1036	N	THR	A	301	10.420	31.980	28.432	1.00	26.55	N
	ATOM	1037	CA	THR	A	301	9.539	33.106	28.142	1.00	27.35	C
	ATOM	1038	C	THR	A	301	8.507	32.672	27.100	1.00	27.20	C
15	ATOM	1039	O	THR	A	301	7.394	33.188	27.069	1.00	27.90	O
	ATOM	1040	CB	THR	A	301	10.324	34.329	27.617	1.00	27.90	C
	ATOM	1041	OG1	THR	A	301	11.097	33.956	26.472	1.00	29.74	O
	ATOM	1042	CG2	THR	A	301	11.250	34.861	28.696	1.00	29.44	C
	ATOM	1043	N	LYS	A	302	8.875	31.715	26.250	1.00	26.49	N
20	ATOM	1044	CA	LYS	A	302	7.948	31.225	25.232	1.00	27.28	C
	ATOM	1045	C	LYS	A	302	6.886	30.318	25.847	1.00	27.81	C
	ATOM	1046	O	LYS	A	302	5.960	29.874	25.160	1.00	27.95	O
	ATOM	1047	CB	LYS	A	302	8.701	30.477	24.130	1.00	28.36	C
	ATOM	1048	CG	LYS	A	302	9.496	31.386	23.206	1.00	29.79	C
25	ATOM	1049	CD	LYS	A	302	10.203	30.586	22.128	1.00	30.72	C
	ATOM	1050	CE	LYS	A	302	11.019	31.482	21.209	1.00	32.93	C
	ATOM	1051	NZ	LYS	A	302	12.121	32.161	21.934	1.00	33.88	N
	ATOM	1052	N	ALA	A	303	7.019	30.048	27.143	1.00	26.44	N
	ATOM	1053	CA	ALA	A	303	6.052	29.219	27.847	1.00	27.88	C
30	ATOM	1054	C	ALA	A	303	5.130	30.097	28.692	1.00	28.91	C
	ATOM	1055	O	ALA	A	303	4.310	29.592	29.457	1.00	29.81	O
	ATOM	1056	CB	ALA	A	303	6.771	28.199	28.726	1.00	27.38	C
	ATOM	1057	N	GLY	A	304	5.279	31.415	28.564	1.00	29.66	N
	ATOM	1058	CA	GLY	A	304	4.423	32.328	29.309	1.00	30.57	C
35	ATOM	1059	C	GLY	A	304	4.963	32.961	30.582	1.00	31.32	C
	ATOM	1060	O	GLY	A	304	4.257	33.735	31.234	1.00	32.07	O
	ATOM	1061	N	HIS	A	305	6.202	32.649	30.948	1.00	31.10	N
	ATOM	1062	CA	HIS	A	305	6.797	33.216	32.155	1.00	30.95	C
	ATOM	1063	C	HIS	A	305	7.656	34.439	31.853	1.00	31.77	C
40	ATOM	1064	O	HIS	A	305	8.138	34.610	30.731	1.00	31.65	O
	ATOM	1065	CB	HIS	A	305	7.628	32.155	32.881	1.00	30.92	C
	ATOM	1066	CG	HIS	A	305	6.799	31.128	33.585	1.00	30.70	C
	ATOM	1067	ND1	HIS	A	305	6.017	31.430	34.679	1.00	31.24	N
	ATOM	1068	CD2	HIS	A	305	6.599	29.812	33.331	1.00	31.47	C
45	ATOM	1069	CE1	HIS	A	305	5.369	30.346	35.067	1.00	31.89	C
	ATOM	1070	NE2	HIS	A	305	5.704	29.351	34.265	1.00	30.48	N
	ATOM	1071	N	SER	A	306	7.839	35.290	32.860	1.00	32.01	N
	ATOM	1072	CA	SER	A	306	8.624	36.511	32.700	1.00	33.97	C
	ATOM	1073	C	SER	A	306	9.982	36.449	33.392	1.00	34.00	C
50	ATOM	1074	O	SER	A	306	10.265	35.523	34.154	1.00	33.09	O
	ATOM	1075	CB	SER	A	306	7.842	37.710	33.235	1.00	34.42	C
	ATOM	1076	OG	SER	A	306	7.739	37.654	34.645	1.00	37.62	O
	ATOM	1077	N	LEU	A	307	10.813	37.455	33.125	1.00	34.07	N
	ATOM	1078	CA	LEU	A	307	12.155	37.537	33.694	1.00	34.93	C
55	ATOM	1079	C	LEU	A	307	12.172	37.666	35.212	1.00	33.80	C
	ATOM	1080	O	LEU	A	307	13.180	37.364	35.851	1.00	33.69	O
	ATOM	1081	CB	LEU	A	307	12.923	38.710	33.068	1.00	36.84	C
	ATOM	1082	CG	LEU	A	307	13.434	38.527	31.634	1.00	39.29	C

-149-

	ATOM	1083	CD1	LEU	A	307	12.282	38.235	30.685	1.00	40.58	C
	ATOM	1084	CD2	LEU	A	307	14.168	39.784	31.201	1.00	40.01	C
	ATOM	1085	N	GLU	A	308	11.060	38.110	35.789	1.00	33.38	N
5	ATOM	1086	CA	GLU	A	308	10.963	38.265	37.235	1.00	32.81	C
	ATOM	1087	C	GLU	A	308	11.165	36.913	37.917	1.00	31.88	C
	ATOM	1088	O	GLU	A	308	11.558	36.842	39.078	1.00	30.22	O
	ATOM	1089	CB	GLU	A	308	9.603	38.856	37.607	1.00	37.03	C
	ATOM	1090	CG	GLU	A	308	9.308	40.169	36.888	1.00	42.70	C
10	ATOM	1091	CD	GLU	A	308	7.914	40.707	37.166	1.00	45.49	C
	ATOM	1092	OE1	GLU	A	308	7.522	41.696	36.507	1.00	46.94	O
	ATOM	1093	OE2	GLU	A	308	7.214	40.149	38.040	1.00	47.58	O
	ATOM	1094	N	LEU	A	309	10.898	35.838	37.182	1.00	29.69	N
	ATOM	1095	CA	LEU	A	309	11.081	34.492	37.714	1.00	29.34	C
15	ATOM	1096	C	LEU	A	309	12.348	33.872	37.130	1.00	28.31	C
	ATOM	1097	O	LEU	A	309	13.160	33.290	37.848	1.00	26.92	O
	ATOM	1098	CB	LEU	A	309	9.882	33.605	37.360	1.00	28.48	C
	ATOM	1099	CG	LEU	A	309	10.037	32.116	37.700	1.00	28.85	C
	ATOM	1100	CD1	LEU	A	309	10.011	31.931	39.211	1.00	29.55	C
20	ATOM	1101	CD2	LEU	A	309	8.919	31.312	37.048	1.00	29.07	C
	ATOM	1102	N	ILE	A	310	12.524	34.019	35.822	1.00	28.87	N
	ATOM	1103	CA	ILE	A	310	13.673	33.428	35.142	1.00	30.36	C
	ATOM	1104	C	ILE	A	310	15.051	33.907	35.590	1.00	30.97	C
	ATOM	1105	O	ILE	A	310	15.948	33.092	35.808	1.00	30.03	O
25	ATOM	1106	CB	ILE	A	310	13.552	33.605	33.617	1.00	31.31	C
	ATOM	1107	CG1	ILE	A	310	12.218	33.023	33.139	1.00	32.43	C
	ATOM	1108	CG2	ILE	A	310	14.695	32.884	32.918	1.00	32.83	C
	ATOM	1109	CD1	ILE	A	310	11.920	33.289	31.681	1.00	33.95	C
	ATOM	1110	N	GLU	A	311	15.240	35.213	35.726	1.00	31.83	N
30	ATOM	1111	CA	GLU	A	311	16.547	35.707	36.151	1.00	33.28	C
	ATOM	1112	C	GLU	A	311	16.945	35.175	37.528	1.00	31.76	C
	ATOM	1113	O	GLU	A	311	18.067	34.707	37.714	1.00	31.24	O
	ATOM	1114	CB	GLU	A	311	16.573	37.237	36.128	1.00	35.65	C
	ATOM	1115	CG	GLU	A	311	16.550	37.788	34.710	1.00	41.13	C
35	ATOM	1116	CD	GLU	A	311	16.753	39.287	34.649	1.00	43.32	C
	ATOM	1117	OE1	GLU	A	311	16.858	39.815	33.522	1.00	46.68	O
	ATOM	1118	OE2	GLU	A	311	16.807	39.933	35.718	1.00	45.68	O
	ATOM	1119	N	PRO	A	312	16.032	35.232	38.511	1.00	30.94	N
	ATOM	1120	CA	PRO	A	312	16.358	34.728	39.851	1.00	29.89	C
40	ATOM	1121	C	PRO	A	312	16.570	33.212	39.817	1.00	28.28	C
	ATOM	1122	O	PRO	A	312	17.321	32.656	40.619	1.00	28.14	O
	ATOM	1123	CB	PRO	A	312	15.132	35.115	40.675	1.00	30.62	C
	ATOM	1124	CG	PRO	A	312	14.612	36.330	39.962	1.00	31.93	C
	ATOM	1125	CD	PRO	A	312	14.740	35.943	38.523	1.00	31.29	C
45	ATOM	1126	N	LEU	A	313	15.896	32.550	38.883	1.00	26.85	N
	ATOM	1127	CA	LEU	A	313	16.013	31.102	38.739	1.00	26.51	C
	ATOM	1128	C	LEU	A	313	17.425	30.764	38.267	1.00	25.16	C
	ATOM	1129	O	LEU	A	313	18.063	29.855	38.788	1.00	24.33	O
	ATOM	1130	CB	LEU	A	313	14.998	30.583	37.715	1.00	27.97	C
	ATOM	1131	CG	LEU	A	313	14.373	29.198	37.935	1.00	31.36	C
50	ATOM	1132	CD1	LEU	A	313	13.860	28.676	36.600	1.00	29.96	C
	ATOM	1133	CD2	LEU	A	313	15.366	28.230	38.536	1.00	30.03	C
	ATOM	1134	N	ILE	A	314	17.917	31.504	37.279	1.00	25.12	N
	ATOM	1135	CA	ILE	A	314	19.262	31.255	36.763	1.00	25.36	C
	ATOM	1136	C	ILE	A	314	20.304	31.552	37.839	1.00	25.44	C
55	ATOM	1137	O	ILE	A	314	21.267	30.802	38.008	1.00	25.07	O
	ATOM	1138	CB	ILE	A	314	19.565	32.122	35.517	1.00	26.51	C
	ATOM	1139	CG1	ILE	A	314	18.560	31.811	34.400	1.00	28.21	C
	ATOM	1140	CG2	ILE	A	314	20.982	31.844	35.028	1.00	26.75	C

-150-

	ATOM	1141	CD1	ILE A 314	18.654	30.407	33.858	1.00	29.90	C
	ATOM	1142	N	LYS A 315	20.112	32.641	38.574	1.00	25.44	N
	ATOM	1143	CA	LYS A 315	21.058	32.994	39.626	1.00	26.52	C
5	ATOM	1144	C	LYS A 315	21.117	31.869	40.656	1.00	25.66	C
	ATOM	1145	O	LYS A 315	22.193	31.522	41.149	1.00	25.67	O
	ATOM	1146	CB	LYS A 315	20.651	34.310	40.296	1.00	28.77	C
	ATOM	1147	CG	LYS A 315	21.759	34.926	41.134	1.00	34.86	C
	ATOM	1148	CD	LYS A 315	21.562	36.427	41.306	1.00	37.34	C
10	ATOM	1149	CE	LYS A 315	22.806	37.082	41.891	1.00	39.12	C
	ATOM	1150	NZ	LYS A 315	23.154	36.521	43.227	1.00	41.56	N
	ATOM	1151	N	PHE A 316	19.958	31.295	40.967	1.00	23.92	N
	ATOM	1152	CA	PHE A 316	19.874	30.196	41.921	1.00	23.22	C
	ATOM	1153	C	PHE A 316	20.662	28.997	41.400	1.00	22.36	C
15	ATOM	1154	O	PHE A 316	21.422	28.380	42.151	1.00	22.35	O
	ATOM	1155	CB	PHE A 316	18.410	29.791	42.144	1.00	24.22	C
	ATOM	1156	CG	PHE A 316	18.242	28.546	42.979	1.00	26.30	C
	ATOM	1157	CD1	PHE A 316	18.323	28.605	44.370	1.00	27.43	C
	ATOM	1158	CD2	PHE A 316	18.037	27.310	42.372	1.00	26.87	C
20	ATOM	1159	CE1	PHE A 316	18.204	27.446	45.141	1.00	28.46	C
	ATOM	1160	CE2	PHE A 316	17.918	26.145	43.135	1.00	27.51	C
	ATOM	1161	CZ	PHE A 316	18.002	26.218	44.520	1.00	28.27	C
	ATOM	1162	N	GLN A 317	20.480	28.665	40.120	1.00	21.28	N
	ATOM	1163	CA	GLN A 317	21.175	27.524	39.522	1.00	21.35	C
25	ATOM	1164	C	GLN A 317	22.694	27.681	39.586	1.00	21.92	C
	ATOM	1165	O	GLN A 317	23.410	26.735	39.913	1.00	20.68	O
	ATOM	1166	CB	GLN A 317	20.754	27.324	38.057	1.00	21.98	C
	ATOM	1167	CG	GLN A 317	19.296	26.891	37.855	1.00	22.78	C
	ATOM	1168	CD	GLN A 317	18.968	25.585	38.563	1.00	25.08	C
30	ATOM	1169	OE1	GLN A 317	19.792	24.670	38.619	1.00	26.08	O
	ATOM	1170	NE2	GLN A 317	17.756	25.488	39.093	1.00	22.14	N
	ATOM	1171	N	VAL A 318	23.188	28.870	39.259	1.00	22.58	N
	ATOM	1172	CA	VAL A 318	24.629	29.108	39.301	1.00	23.76	C
	ATOM	1173	C	VAL A 318	25.162	28.983	40.734	1.00	24.71	C
35	ATOM	1174	O	VAL A 318	26.199	28.349	40.971	1.00	26.38	O
	ATOM	1175	CB	VAL A 318	24.975	30.510	38.727	1.00	24.56	C
	ATOM	1176	CG1	VAL A 318	26.458	30.798	38.897	1.00	26.05	C
	ATOM	1177	CG2	VAL A 318	24.608	30.567	37.255	1.00	23.60	C
	ATOM	1178	N	GLY A 319	24.447	29.574	41.687	1.00	25.34	N
40	ATOM	1179	CA	GLY A 319	24.868	29.515	43.076	1.00	26.42	C
	ATOM	1180	C	GLY A 319	24.892	28.099	43.623	1.00	26.70	C
	ATOM	1181	O	GLY A 319	25.778	27.738	44.399	1.00	26.15	O
	ATOM	1182	N	LEU A 320	23.915	27.292	43.226	1.00	25.08	N
	ATOM	1183	CA	LEU A 320	23.856	25.910	43.680	1.00	26.49	C
45	ATOM	1184	C	LEU A 320	25.001	25.141	43.019	1.00	26.16	C
	ATOM	1185	O	LEU A 320	25.674	24.342	43.666	1.00	25.62	O
	ATOM	1186	CB	LEU A 320	22.499	25.289	43.318	1.00	26.17	C
	ATOM	1187	CG	LEU A 320	22.202	23.895	43.877	1.00	29.00	C
	ATOM	1188	CD1	LEU A 320	22.305	23.911	45.394	1.00	28.44	C
	ATOM	1189	CD2	LEU A 320	20.803	23.457	43.439	1.00	27.28	C
50	ATOM	1190	N	LYS A 321	25.231	25.402	41.734	1.00	26.97	N
	ATOM	1191	CA	LYS A 321	26.312	24.743	41.000	1.00	29.33	C
	ATOM	1192	C	LYS A 321	27.664	24.983	41.649	1.00	30.36	C
	ATOM	1193	O	LYS A 321	28.486	24.070	41.746	1.00	30.00	O
55	ATOM	1194	CB	LYS A 321	26.385	25.252	39.561	1.00	30.33	C
	ATOM	1195	CG	LYS A 321	25.578	24.465	38.559	1.00	33.36	C
	ATOM	1196	CD	LYS A 321	26.140	23.069	38.341	1.00	33.34	C
	ATOM	1197	CE	LYS A 321	25.279	22.329	37.336	1.00	33.36	C
	ATOM	1198	NZ	LYS A 321	25.668	20.911	37.111	1.00	32.77	N

-151-

	ATOM	1199	N	LYS	A	322	27.894	26.222	42.077	1.00	30.82	N
	ATOM	1200	CA	LYS	A	322	29.155	26.601	42.702	1.00	32.19	C
	ATOM	1201	C	LYS	A	322	29.447	25.934	44.037	1.00	32.03	C
5	ATOM	1202	O	LYS	A	322	30.598	25.896	44.462	1.00	32.87	O
	ATOM	1203	CB	LYS	A	322	29.234	28.122	42.866	1.00	33.78	C
	ATOM	1204	CG	LYS	A	322	29.592	28.853	41.587	1.00	37.24	C
	ATOM	1205	CD	LYS	A	322	29.849	30.328	41.856	1.00	39.61	C
	ATOM	1206	CE	LYS	A	322	30.611	30.964	40.712	1.00	41.25	C
10	ATOM	1207	NZ	LYS	A	322	31.956	30.335	40.544	1.00	43.80	N
	ATOM	1208	N	LEU	A	323	28.420	25.415	44.703	1.00	30.51	N
	ATOM	1209	CA	LEU	A	323	28.627	24.747	45.985	1.00	31.09	C
	ATOM	1210	C	LEU	A	323	29.296	23.392	45.774	1.00	31.05	C
	ATOM	1211	O	LEU	A	323	29.833	22.805	46.715	1.00	31.05	O
15	ATOM	1212	CB	LEU	A	323	27.297	24.544	46.719	1.00	30.29	C
	ATOM	1213	CG	LEU	A	323	26.551	25.784	47.220	1.00	31.62	C
	ATOM	1214	CD1	LEU	A	323	25.260	25.359	47.904	1.00	30.41	C
	ATOM	1215	CD2	LEU	A	323	27.434	26.570	48.180	1.00	31.32	C
	ATOM	1216	N	ASN	A	324	29.264	22.908	44.535	1.00	30.91	N
20	ATOM	1217	CA	ASN	A	324	29.854	21.619	44.180	1.00	32.42	C
	ATOM	1218	C	ASN	A	324	29.466	20.524	45.165	1.00	32.07	C
	ATOM	1219	O	ASN	A	324	30.323	19.864	45.755	1.00	32.62	O
	ATOM	1220	CB	ASN	A	324	31.380	21.722	44.110	1.00	36.14	C
	ATOM	1221	CG	ASN	A	324	31.853	22.576	42.954	1.00	38.53	C
25	ATOM	1222	OD1	ASN	A	324	32.013	23.789	43.087	1.00	43.04	O
	ATOM	1223	ND2	ASN	A	324	32.068	21.947	41.805	1.00	40.87	N
	ATOM	1224	N	LEU	A	325	28.166	20.326	45.333	1.00	29.80	N
	ATOM	1225	CA	LEU	A	325	27.667	19.320	46.257	1.00	27.98	C
	ATOM	1226	C	LEU	A	325	27.969	17.890	45.836	1.00	27.42	C
30	ATOM	1227	O	LEU	A	325	27.984	17.568	44.648	1.00	27.50	O
	ATOM	1228	CB	LEU	A	325	26.149	19.454	46.409	1.00	28.15	C
	ATOM	1229	CG	LEU	A	325	25.592	20.785	46.907	1.00	28.88	C
	ATOM	1230	CD1	LEU	A	325	24.072	20.701	46.960	1.00	29.23	C
	ATOM	1231	CD2	LEU	A	325	26.163	21.105	48.276	1.00	28.09	C
35	ATOM	1232	N	HIS	A	326	28.219	17.033	46.821	1.00	26.59	N
	ATOM	1233	CA	HIS	A	326	28.430	15.618	46.546	1.00	25.79	C
	ATOM	1234	C	HIS	A	326	27.003	15.162	46.264	1.00	25.33	C
	ATOM	1235	O	HIS	A	326	26.052	15.819	46.695	1.00	23.44	O
	ATOM	1236	CB	HIS	A	326	28.935	14.882	47.788	1.00	27.17	C
40	ATOM	1237	CG	HIS	A	326	30.303	15.294	48.231	1.00	27.36	C
	ATOM	1238	ND1	HIS	A	326	30.942	14.704	49.301	1.00	28.09	N
	ATOM	1239	CD2	HIS	A	326	31.159	16.222	47.744	1.00	28.85	C
	ATOM	1240	CE1	HIS	A	326	32.135	15.251	49.453	1.00	28.02	C
	ATOM	1241	NE2	HIS	A	326	32.292	16.174	48.521	1.00	29.20	N
45	ATOM	1242	N	GLU	A	327	26.839	14.054	45.554	1.00	24.49	N
	ATOM	1243	CA	GLU	A	327	25.497	13.569	45.267	1.00	24.94	C
	ATOM	1244	C	GLU	A	327	24.768	13.297	46.583	1.00	24.29	C
	ATOM	1245	O	GLU	A	327	23.553	13.498	46.686	1.00	24.42	O
	ATOM	1246	CB	GLU	A	327	25.557	12.302	44.409	1.00	27.30	C
50	ATOM	1247	CG	GLU	A	327	24.185	11.755	44.032	1.00	29.69	C
	ATOM	1248	CD	GLU	A	327	24.247	10.740	42.903	1.00	32.63	C
	ATOM	1249	OE1	GLU	A	327	25.021	9.771	43.015	1.00	31.56	O
	ATOM	1250	OE2	GLU	A	327	23.519	10.915	41.903	1.00	32.79	O
	ATOM	1251	N	GLU	A	328	25.516	12.858	47.595	1.00	22.79	N
55	ATOM	1252	CA	GLU	A	328	24.942	12.576	48.911	1.00	23.11	C
	ATOM	1253	C	GLU	A	328	24.280	13.822	49.500	1.00	23.46	C
	ATOM	1254	O	GLU	A	328	23.199	13.750	50.086	1.00	23.51	O
	ATOM	1255	CB	GLU	A	328	26.025	12.083	49.877	1.00	24.71	C
	ATOM	1256	CG	GLU	A	328	26.540	10.666	49.607	1.00	25.97	C

-152-

	ATOM	1257	CD	GLU	A	328	27.584	10.591	48.506	1.00	28.78	C
	ATOM	1258	OE1	GLU	A	328	28.201	9.512	48.356	1.00	29.81	O
	ATOM	1259	OE2	GLU	A	328	27.793	11.591	47.789	1.00	27.61	O
5	ATOM	1260	N	GLU	A	329	24.939	14.965	49.349	1.00	22.58	N
	ATOM	1261	CA	GLU	A	329	24.406	16.221	49.861	1.00	23.12	C
	ATOM	1262	C	GLU	A	329	23.212	16.678	49.026	1.00	22.73	C
	ATOM	1263	O	GLU	A	329	22.236	17.203	49.558	1.00	22.26	O
	ATOM	1264	CB	GLU	A	329	25.511	17.281	49.856	1.00	23.27	C
10	ATOM	1265	CG	GLU	A	329	26.608	16.943	50.859	1.00	24.71	C
	ATOM	1266	CD	GLU	A	329	27.940	17.599	50.554	1.00	26.09	C
	ATOM	1267	OE1	GLU	A	329	28.825	17.532	51.429	1.00	27.57	O
	ATOM	1268	OE2	GLU	A	329	28.113	18.160	49.454	1.00	26.68	O
	ATOM	1269	N	HIS	A	330	23.291	16.450	47.721	1.00	22.72	N
15	ATOM	1270	CA	HIS	A	330	22.225	16.836	46.803	1.00	22.97	C
	ATOM	1271	C	HIS	A	330	20.908	16.139	47.150	1.00	23.43	C
	ATOM	1272	O	HIS	A	330	19.863	16.790	47.257	1.00	22.10	O
	ATOM	1273	CB	HIS	A	330	22.638	16.494	45.364	1.00	24.13	C
	ATOM	1274	CG	HIS	A	330	21.648	16.916	44.321	1.00	25.22	C
	ATOM	1275	ND1	HIS	A	330	21.357	18.237	44.060	1.00	25.99	N
20	ATOM	1276	CD2	HIS	A	330	20.913	16.190	43.444	1.00	25.76	C
	ATOM	1277	CE1	HIS	A	330	20.489	18.307	43.065	1.00	26.73	C
	ATOM	1278	NE2	HIS	A	330	20.203	17.078	42.674	1.00	25.08	N
	ATOM	1279	N	VAL	A	331	20.955	14.823	47.334	1.00	22.22	N
25	ATOM	1280	CA	VAL	A	331	19.739	14.072	47.642	1.00	23.00	C
	ATOM	1281	C	VAL	A	331	19.185	14.382	49.024	1.00	22.12	C
	ATOM	1282	O	VAL	A	331	17.968	14.393	49.218	1.00	21.17	O
	ATOM	1283	CB	VAL	A	331	19.952	12.544	47.490	1.00	22.74	C
	ATOM	1284	CG1	VAL	A	331	20.363	12.233	46.053	1.00	25.60	C
	ATOM	1285	CG2	VAL	A	331	21.008	12.045	48.466	1.00	25.97	C
30	ATOM	1286	N	LEU	A	332	20.067	14.634	49.986	1.00	21.61	N
	ATOM	1287	CA	LEU	A	332	19.611	14.967	51.327	1.00	21.81	C
	ATOM	1288	C	LEU	A	332	18.884	16.311	51.301	1.00	21.82	C
	ATOM	1289	O	LEU	A	332	17.874	16.489	51.976	1.00	22.23	O
35	ATOM	1290	CB	LEU	A	332	20.796	15.020	52.303	1.00	22.40	C
	ATOM	1291	CG	LEU	A	332	21.262	13.656	52.824	1.00	22.71	C
	ATOM	1292	CD1	LEU	A	332	22.617	13.777	53.516	1.00	23.21	C
	ATOM	1293	CD2	LEU	A	332	20.214	13.112	53.776	1.00	23.85	C
	ATOM	1294	N	LEU	A	333	19.389	17.253	50.508	1.00	21.45	N
	ATOM	1295	CA	LEU	A	333	18.763	18.569	50.420	1.00	22.43	C
40	ATOM	1296	C	LEU	A	333	17.363	18.478	49.808	1.00	21.61	C
	ATOM	1297	O	LEU	A	333	16.440	19.157	50.259	1.00	21.39	O
	ATOM	1298	CB	LEU	A	333	19.637	19.521	49.599	1.00	23.63	C
	ATOM	1299	CG	LEU	A	333	19.221	21.000	49.597	1.00	26.05	C
	ATOM	1300	CD1	LEU	A	333	19.253	21.557	51.014	1.00	26.27	C
45	ATOM	1301	CD2	LEU	A	333	20.157	21.785	48.703	1.00	26.03	C
	ATOM	1302	N	MET	A	334	17.198	17.654	48.776	1.00	21.27	N
	ATOM	1303	CA	MET	A	334	15.878	17.513	48.163	1.00	20.93	C
	ATOM	1304	C	MET	A	334	14.928	16.881	49.171	1.00	21.48	C
	ATOM	1305	O	MET	A	334	13.769	17.263	49.256	1.00	21.52	O
50	ATOM	1306	CB	MET	A	334	15.939	16.648	46.896	1.00	21.53	C
	ATOM	1307	CG	MET	A	334	16.631	17.318	45.719	1.00	22.31	C
	ATOM	1308	SD	MET	A	334	16.442	16.343	44.219	1.00	24.84	S
	ATOM	1309	CE	MET	A	334	17.484	14.909	44.612	1.00	24.19	C
	ATOM	1310	N	ALA	A	335	15.427	15.922	49.950	1.00	21.64	N
55	ATOM	1311	CA	ALA	A	335	14.596	15.255	50.949	1.00	21.82	C
	ATOM	1312	C	ALA	A	335	14.167	16.231	52.045	1.00	22.81	C
	ATOM	1313	O	ALA	A	335	13.002	16.248	52.455	1.00	22.95	O
	ATOM	1314	CB	ALA	A	335	15.355	14.070	51.564	1.00	22.44	C

-153-

	ATOM	1315	N	ILE A 336	15.111	17.041	52.517	1.00	21.90	N
	ATOM	1316	CA	ILE A 336	14.827	18.022	53.560	1.00	22.98	C
	ATOM	1317	C	ILE A 336	13.822	19.050	53.038	1.00	23.92	C
5	ATOM	1318	O	ILE A 336	12.949	19.496	53.772	1.00	23.55	O
	ATOM	1319	CB	ILE A 336	16.129	18.730	54.020	1.00	23.77	C
	ATOM	1320	CG1	ILE A 336	17.021	17.724	54.753	1.00	24.24	C
	ATOM	1321	CG2	ILE A 336	15.803	19.914	54.936	1.00	25.02	C
	ATOM	1322	CD1	ILE A 336	18.445	18.188	54.950	1.00	27.51	C
10	ATOM	1323	N	CYS A 337	13.942	19.411	51.765	1.00	22.82	N
	ATOM	1324	CA	CYS A 337	13.020	20.365	51.166	1.00	23.92	C
	ATOM	1325	C	CYS A 337	11.582	19.846	51.235	1.00	24.00	C
	ATOM	1326	O	CYS A 337	10.665	20.577	51.605	1.00	25.45	O
	ATOM	1327	CB	CYS A 337	13.410	20.622	49.705	1.00	22.95	C
15	ATOM	1328	SG	CYS A 337	12.289	21.736	48.817	1.00	25.85	S
	ATOM	1329	N	ILE A 338	11.393	18.578	50.886	1.00	23.65	N
	ATOM	1330	CA	ILE A 338	10.070	17.957	50.890	1.00	23.56	C
	ATOM	1331	C	ILE A 338	9.457	17.814	52.284	1.00	26.02	C
	ATOM	1332	O	ILE A 338	8.288	18.153	52.501	1.00	25.70	O
20	ATOM	1333	CB	ILE A 338	10.126	16.560	50.231	1.00	23.28	C
	ATOM	1334	CG1	ILE A 338	10.483	16.704	48.746	1.00	22.98	C
	ATOM	1335	CG2	ILE A 338	8.794	15.839	50.396	1.00	24.00	C
	ATOM	1336	CD1	ILE A 338	10.807	15.387	48.057	1.00	22.98	C
	ATOM	1337	N	VAL A 339	10.242	17.305	53.225	1.00	26.29	N
25	ATOM	1338	CA	VAL A 339	9.754	17.106	54.584	1.00	29.21	C
	ATOM	1339	C	VAL A 339	9.971	18.359	55.430	1.00	29.45	C
	ATOM	1340	O	VAL A 339	10.807	18.378	56.333	1.00	30.57	O
	ATOM	1341	CB	VAL A 339	10.461	15.901	55.241	1.00	30.37	C
	ATOM	1342	CG1	VAL A 339	9.751	15.516	56.524	1.00	31.20	C
30	ATOM	1343	CG2	VAL A 339	10.479	14.725	54.277	1.00	31.68	C
	ATOM	1344	N	SER A 340	9.213	19.407	55.122	1.00	30.04	N
	ATOM	1345	CA	SER A 340	9.309	20.676	55.842	1.00	30.94	C
	ATOM	1346	C	SER A 340	8.061	20.868	56.701	1.00	31.69	C
	ATOM	1347	O	SER A 340	6.940	20.841	56.195	1.00	31.64	O
35	ATOM	1348	CB	SER A 340	9.438	21.838	54.853	1.00	32.39	C
	ATOM	1349	OG	SER A 340	10.664	21.773	54.142	1.00	35.78	O
	ATOM	1350	N	PRO A 341	8.243	21.075	58.013	1.00	32.38	N
	ATOM	1351	CA	PRO A 341	7.107	21.263	58.919	1.00	33.82	C
	ATOM	1352	C	PRO A 341	6.344	22.579	58.774	1.00	35.40	C
40	ATOM	1353	O	PRO A 341	5.204	22.688	59.232	1.00	36.23	O
	ATOM	1354	CB	PRO A 341	7.745	21.111	60.298	1.00	33.68	C
	ATOM	1355	CG	PRO A 341	9.110	21.675	60.094	1.00	33.78	C
	ATOM	1356	CD	PRO A 341	9.517	21.088	58.754	1.00	32.78	C
	ATOM	1357	N	ASP A 342	6.954	23.570	58.131	1.00	36.36	N
45	ATOM	1358	CA	ASP A 342	6.301	24.866	57.981	1.00	37.82	C
	ATOM	1359	C	ASP A 342	5.580	25.094	56.657	1.00	38.30	C
	ATOM	1360	O	ASP A 342	5.655	26.181	56.084	1.00	39.93	O
	ATOM	1361	CB	ASP A 342	7.304	26.001	58.213	1.00	39.62	C
	ATOM	1362	CG	ASP A 342	8.441	25.987	57.218	1.00	41.16	C
50	ATOM	1363	OD1	ASP A 342	9.185	26.989	57.152	1.00	43.27	O
	ATOM	1364	OD2	ASP A 342	8.597	24.974	56.505	1.00	42.71	O
	ATOM	1365	N	ARG A 343	4.887	24.072	56.170	1.00	37.31	N
	ATOM	1366	CA	ARG A 343	4.123	24.195	54.933	1.00	37.10	C
	ATOM	1367	C	ARG A 343	2.683	24.409	55.375	1.00	37.98	C
55	ATOM	1368	O	ARG A 343	2.198	23.723	56.273	1.00	38.15	O
	ATOM	1369	CB	ARG A 343	4.207	22.911	54.103	1.00	35.71	C
	ATOM	1370	CG	ARG A 343	5.595	22.543	53.612	1.00	32.83	C
	ATOM	1371	CD	ARG A 343	6.123	23.513	52.565	1.00	31.70	C
	ATOM	1372	NE	ARG A 343	7.282	22.947	51.879	1.00	29.77	N

-154-

	ATOM	1373	CZ	ARG A 343	8.062	23.612	51.032	1.00	28.95	C
	ATOM	1374	NH1	ARG A 343	7.818	24.886	50.751	1.00	27.66	N
	ATOM	1375	NH2	ARG A 343	9.097	23.002	50.472	1.00	28.12	N
5	ATOM	1376	N	PRO A 344	1.979	25.367	54.761	1.00	39.05	N
	ATOM	1377	CA	PRO A 344	0.592	25.579	55.180	1.00	39.38	C
	ATOM	1378	C	PRO A 344	-0.279	24.351	54.924	1.00	38.87	C
	ATOM	1379	O	PRO A 344	-0.205	23.742	53.858	1.00	39.29	O
	ATOM	1380	CB	PRO A 344	0.167	26.786	54.348	1.00	39.90	C
10	ATOM	1381	CG	PRO A 344	0.974	26.624	53.092	1.00	40.56	C
	ATOM	1382	CD	PRO A 344	2.332	26.243	53.630	1.00	39.66	C
	ATOM	1383	N	GLY A 345	-1.085	23.978	55.912	1.00	38.50	N
	ATOM	1384	CA	GLY A 345	-1.965	22.836	55.746	1.00	37.96	C
	ATOM	1385	C	GLY A 345	-1.567	21.544	56.437	1.00	37.94	C
	ATOM	1386	O	GLY A 345	-2.386	20.630	56.537	1.00	36.75	O
15	ATOM	1387	N	VAL A 346	-0.328	21.452	56.914	1.00	37.90	N
	ATOM	1388	CA	VAL A 346	0.125	20.234	57.585	1.00	38.39	C
	ATOM	1389	C	VAL A 346	-0.584	20.046	58.922	1.00	39.30	C
	ATOM	1390	O	VAL A 346	-0.832	21.012	59.643	1.00	39.35	O
20	ATOM	1391	CB	VAL A 346	1.654	20.249	57.827	1.00	38.81	C
	ATOM	1392	CG1	VAL A 346	2.383	20.409	56.503	1.00	37.92	C
	ATOM	1393	CG2	VAL A 346	2.030	21.366	58.784	1.00	38.02	C
	ATOM	1394	N	GLN A 347	-0.905	18.796	59.247	1.00	39.79	N
	ATOM	1395	CA	GLN A 347	-1.597	18.481	60.492	1.00	40.19	C
	ATOM	1396	C	GLN A 347	-0.631	18.135	61.612	1.00	38.86	C
25	ATOM	1397	O	GLN A 347	-0.657	18.758	62.673	1.00	39.58	O
	ATOM	1398	CB	GLN A 347	-2.564	17.314	60.280	1.00	43.00	C
	ATOM	1399	CG	GLN A 347	-3.565	17.531	59.157	1.00	47.50	C
	ATOM	1400	CD	GLN A 347	-4.526	18.678	59.423	1.00	50.27	C
30	ATOM	1401	OE1	GLN A 347	-4.582	19.209	60.535	1.00	52.52	O
	ATOM	1402	NE2	GLN A 347	-5.283	19.071	58.402	1.00	51.48	N
	ATOM	1403	N	ASP A 348	0.223	17.144	61.380	1.00	36.34	N
	ATOM	1404	CA	ASP A 348	1.181	16.730	62.398	1.00	35.34	C
	ATOM	1405	C	ASP A 348	2.568	17.313	62.152	1.00	33.83	C
	ATOM	1406	O	ASP A 348	3.474	16.622	61.679	1.00	33.85	O
35	ATOM	1407	CB	ASP A 348	1.257	15.203	62.458	1.00	34.84	C
	ATOM	1408	CG	ASP A 348	1.947	14.707	63.712	1.00	35.23	C
	ATOM	1409	OD1	ASP A 348	1.907	13.488	63.972	1.00	34.74	O
	ATOM	1410	OD2	ASP A 348	2.531	15.539	64.437	1.00	34.97	O
40	ATOM	1411	N	ALA A 349	2.727	18.587	62.492	1.00	32.41	N
	ATOM	1412	CA	ALA A 349	3.991	19.286	62.307	1.00	32.51	C
	ATOM	1413	C	ALA A 349	5.122	18.665	63.121	1.00	32.68	C
	ATOM	1414	O	ALA A 349	6.263	18.602	62.662	1.00	32.47	O
	ATOM	1415	CB	ALA A 349	3.829	20.753	62.677	1.00	32.86	C
45	ATOM	1416	N	ALA A 350	4.804	18.206	64.328	1.00	31.95	N
	ATOM	1417	CA	ALA A 350	5.809	17.602	65.200	1.00	31.15	C
	ATOM	1418	C	ALA A 350	6.458	16.367	64.578	1.00	30.76	C
	ATOM	1419	O	ALA A 350	7.676	16.190	64.655	1.00	30.22	O
	ATOM	1420	CB	ALA A 350	5.180	17.240	66.547	1.00	32.37	C
50	ATOM	1421	N	LEU A 351	5.643	15.510	63.972	1.00	30.64	N
	ATOM	1422	CA	LEU A 351	6.150	14.298	63.340	1.00	30.92	C
	ATOM	1423	C	LEU A 351	7.032	14.690	62.156	1.00	30.72	C
	ATOM	1424	O	LEU A 351	8.137	14.181	61.995	1.00	30.35	O
	ATOM	1425	CB	LEU A 351	4.989	13.428	62.848	1.00	32.92	C
	ATOM	1426	CG	LEU A 351	5.214	11.919	62.690	1.00	34.73	C
55	ATOM	1427	CD1	LEU A 351	4.073	11.326	61.881	1.00	35.25	C
	ATOM	1428	CD2	LEU A 351	6.528	11.640	62.005	1.00	36.86	C
	ATOM	1429	N	ILE A 352	6.531	15.597	61.325	1.00	30.54	N
	ATOM	1430	CA	ILE A 352	7.282	16.056	60.158	1.00	29.35	C

-155-

	ATOM	1431	C	ILE A 352	8.628	16.646	60.580	1.00	29.73	C
	ATOM	1432	O	ILE A 352	9.658	16.371	59.959	1.00	30.37	O
	ATOM	1433	CB	ILE A 352	6.465	17.107	59.362	1.00	29.44	C
5	ATOM	1434	CG1	ILE A 352	5.175	16.463	58.842	1.00	29.58	C
	ATOM	1435	CG2	ILE A 352	7.290	17.647	58.193	1.00	28.41	C
	ATOM	1436	CD1	ILE A 352	4.166	17.452	58.284	1.00	29.04	C
	ATOM	1437	N	GLU A 353	8.626	17.445	61.644	1.00	30.02	N
	ATOM	1438	CA	GLU A 353	9.857	18.058	62.130	1.00	30.56	C
10	ATOM	1439	C	GLU A 353	10.845	17.000	62.613	1.00	29.99	C
	ATOM	1440	O	GLU A 353	12.050	17.147	62.438	1.00	29.97	O
	ATOM	1441	CB	GLU A 353	9.565	19.048	63.266	1.00	32.59	C
	ATOM	1442	CG	GLU A 353	10.755	19.941	63.615	1.00	35.81	C
	ATOM	1443	CD	GLU A 353	10.462	20.922	64.740	1.00	38.69	C
15	ATOM	1444	OE1	GLU A 353	9.381	21.551	64.723	1.00	40.67	O
	ATOM	1445	OE2	GLU A 353	11.321	21.075	65.637	1.00	40.80	O
	ATOM	1446	N	ALA A 354	10.334	15.935	63.223	1.00	29.90	N
	ATOM	1447	CA	ALA A 354	11.191	14.861	63.716	1.00	29.96	C
	ATOM	1448	C	ALA A 354	11.871	14.191	62.531	1.00	29.90	C
20	ATOM	1449	O	ALA A 354	13.064	13.904	62.570	1.00	31.40	O
	ATOM	1450	CB	ALA A 354	10.367	13.843	64.491	1.00	30.18	C
	ATOM	1451	N	ILE A 355	11.100	13.940	61.478	1.00	29.82	N
	ATOM	1452	CA	ILE A 355	11.638	13.314	60.274	1.00	28.57	C
	ATOM	1453	C	ILE A 355	12.687	14.220	59.628	1.00	28.03	C
25	ATOM	1454	O	ILE A 355	13.754	13.756	59.234	1.00	27.72	O
	ATOM	1455	CB	ILE A 355	10.514	13.022	59.259	1.00	29.38	C
	ATOM	1456	CG1	ILE A 355	9.516	12.036	59.872	1.00	30.07	C
	ATOM	1457	CG2	ILE A 355	11.101	12.458	57.964	1.00	30.16	C
	ATOM	1458	CD1	ILE A 355	8.251	11.849	59.054	1.00	30.83	C
30	ATOM	1459	N	GLN A 356	12.398	15.515	59.534	1.00	27.45	N
	ATOM	1460	CA	GLN A 356	13.345	16.444	58.925	1.00	28.48	C
	ATOM	1461	C	GLN A 356	14.621	16.566	59.754	1.00	29.24	C
	ATOM	1462	O	GLN A 356	15.719	16.622	59.202	1.00	27.50	O
	ATOM	1463	CB	GLN A 356	12.718	17.833	58.739	1.00	28.93	C
35	ATOM	1464	CG	GLN A 356	13.536	18.753	57.823	1.00	29.68	C
	ATOM	1465	CD	GLN A 356	13.064	20.198	57.844	1.00	31.36	C
	ATOM	1466	OE1	GLN A 356	12.996	20.823	58.903	1.00	31.51	O
	ATOM	1467	NE2	GLN A 356	12.747	20.742	56.667	1.00	30.04	N
	ATOM	1468	N	ASP A 357	14.482	16.613	61.078	1.00	29.52	N
40	ATOM	1469	CA	ASP A 357	15.656	16.724	61.945	1.00	30.44	C
	ATOM	1470	C	ASP A 357	16.610	15.550	61.739	1.00	29.70	C
	ATOM	1471	O	ASP A 357	17.827	15.729	61.727	1.00	30.37	O
	ATOM	1472	CB	ASP A 357	15.244	16.791	63.423	1.00	32.83	C
	ATOM	1473	CG	ASP A 357	14.665	18.141	63.812	1.00	34.76	C
45	ATOM	1474	OD1	ASP A 357	14.821	19.110	63.040	1.00	36.63	O
	ATOM	1475	OD2	ASP A 357	14.065	18.236	64.905	1.00	36.89	O
	ATOM	1476	N	ARG A 358	16.059	14.351	61.577	1.00	30.08	N
	ATOM	1477	CA	ARG A 358	16.887	13.167	61.368	1.00	30.11	C
	ATOM	1478	C	ARG A 358	17.689	13.309	60.073	1.00	29.92	C
50	ATOM	1479	O	ARG A 358	18.842	12.880	59.996	1.00	29.08	O
	ATOM	1480	CB	ARG A 358	16.014	11.906	61.323	1.00	31.17	C
	ATOM	1481	CG	ARG A 358	16.796	10.608	61.149	1.00	33.90	C
	ATOM	1482	CD	ARG A 358	15.919	9.382	61.402	1.00	36.03	C
	ATOM	1483	NE	ARG A 358	14.788	9.299	60.479	1.00	38.00	N
55	ATOM	1484	CZ	ARG A 358	13.851	8.358	60.533	1.00	39.39	C
	ATOM	1485	NH1	ARG A 358	13.909	7.417	61.469	1.00	39.22	N
	ATOM	1486	NH2	ARG A 358	12.858	8.353	59.653	1.00	39.21	N
	ATOM	1487	N	LEU A 359	17.074	13.919	59.061	1.00	28.41	N
	ATOM	1488	CA	LEU A 359	17.735	14.128	57.776	1.00	27.76	C

-156-

	ATOM	1489	C	LEU A 359	18.757	15.255	57.890	1.00	27.89	C
	ATOM	1490	O	LEU A 359	19.853	15.171	57.338	1.00	27.13	O
	ATOM	1491	CB	LEU A 359	16.704	14.482	56.697	1.00	27.85	C
	ATOM	1492	CG	LEU A 359	15.646	13.421	56.384	1.00	27.95	C
5	ATOM	1493	CD1	LEU A 359	14.593	13.994	55.448	1.00	28.15	C
	ATOM	1494	CD2	LEU A 359	16.310	12.210	55.758	1.00	28.81	C
	ATOM	1495	N	SER A 360	18.393	16.312	58.610	1.00	28.62	N
	ATOM	1496	CA	SER A 360	19.288	17.448	58.790	1.00	30.04	C
10	ATOM	1497	C	SER A 360	20.540	17.046	59.561	1.00	30.70	C
	ATOM	1498	O	SER A 360	21.647	17.454	59.212	1.00	31.03	O
	ATOM	1499	CB	SER A 360	18.573	18.578	59.534	1.00	32.12	C
	ATOM	1500	OG	SER A 360	17.496	19.084	58.765	1.00	36.13	O
	ATOM	1501	N	ASN A 361	20.367	16.251	60.613	1.00	31.34	N
15	ATOM	1502	CA	ASN A 361	21.513	15.816	61.405	1.00	31.58	C
	ATOM	1503	C	ASN A 361	22.417	14.921	60.570	1.00	30.77	C
	ATOM	1504	O	ASN A 361	23.637	14.935	60.728	1.00	31.06	O
	ATOM	1505	CB	ASN A 361	21.055	15.083	62.667	1.00	34.28	C
	ATOM	1506	CG	ASN A 361	20.328	15.998	63.637	1.00	37.26	C
20	ATOM	1507	OD1	ASN A 361	20.736	17.139	63.854	1.00	39.61	O
	ATOM	1508	ND2	ASN A 361	19.252	15.497	64.234	1.00	39.64	N
	ATOM	1509	N	THR A 362	21.815	14.146	59.674	1.00	29.26	N
	ATOM	1510	CA	THR A 362	22.583	13.270	58.800	1.00	28.14	C
	ATOM	1511	C	THR A 362	23.419	14.135	57.863	1.00	27.56	C
25	ATOM	1512	O	THR A 362	24.607	13.879	57.654	1.00	27.15	O
	ATOM	1513	CB	THR A 362	21.654	12.371	57.956	1.00	28.47	C
	ATOM	1514	OG1	THR A 362	20.923	11.495	58.823	1.00	28.00	O
	ATOM	1515	CG2	THR A 362	22.461	11.548	56.955	1.00	27.60	C
	ATOM	1516	N	LEU A 363	22.795	15.167	57.301	1.00	26.97	N
30	ATOM	1517	CA	LEU A 363	23.493	16.064	56.388	1.00	27.40	C
	ATOM	1518	C	LEU A 363	24.623	16.798	57.100	1.00	28.23	C
	ATOM	1519	O	LEU A 363	25.736	16.884	56.588	1.00	27.96	O
	ATOM	1520	CB	LEU A 363	22.519	17.089	55.782	1.00	26.59	C
	ATOM	1521	CG	LEU A 363	23.153	18.156	54.882	1.00	26.54	C
35	ATOM	1522	CD1	LEU A 363	23.829	17.495	53.687	1.00	26.43	C
	ATOM	1523	CD2	LEU A 363	22.090	19.142	54.417	1.00	26.28	C
	ATOM	1524	N	GLN A 364	24.340	17.325	58.286	1.00	29.48	N
	ATOM	1525	CA	GLN A 364	25.360	18.054	59.029	1.00	31.77	C
	ATOM	1526	C	GLN A 364	26.530	17.140	59.399	1.00	30.91	C
40	ATOM	1527	O	GLN A 364	27.691	17.539	59.307	1.00	30.91	O
	ATOM	1528	CB	GLN A 364	24.747	18.681	60.283	1.00	33.97	C
	ATOM	1529	CG	GLN A 364	25.579	19.812	60.870	1.00	39.97	C
	ATOM	1530	CD	GLN A 364	24.749	20.793	61.681	1.00	41.73	C
	ATOM	1531	OE1	GLN A 364	25.270	21.785	62.190	1.00	45.56	O
45	ATOM	1532	NE2	GLN A 364	23.452	20.523	61.800	1.00	43.48	N
	ATOM	1533	N	THR A 365	26.224	15.910	59.799	1.00	30.38	N
	ATOM	1534	CA	THR A 365	27.263	14.956	60.176	1.00	30.54	C
	ATOM	1535	C	THR A 365	28.099	14.561	58.965	1.00	29.67	C
	ATOM	1536	O	THR A 365	29.319	14.454	59.054	1.00	30.84	O
50	ATOM	1537	CB	THR A 365	26.658	13.687	60.802	1.00	30.66	C
	ATOM	1538	OG1	THR A 365	25.883	14.045	61.952	1.00	32.31	O
	ATOM	1539	CG2	THR A 365	27.759	12.728	61.225	1.00	31.16	C
	ATOM	1540	N	TYR A 366	27.437	14.348	57.832	1.00	29.11	N
	ATOM	1541	CA	TYR A 366	28.131	13.976	56.606	1.00	28.71	C
55	ATOM	1542	C	TYR A 366	29.123	15.051	56.167	1.00	28.75	C
	ATOM	1543	O	TYR A 366	30.261	14.746	55.826	1.00	29.49	O
	ATOM	1544	CB	TYR A 366	27.122	13.708	55.476	1.00	27.69	C
	ATOM	1545	CG	TYR A 366	27.779	13.396	54.148	1.00	27.26	C
	ATOM	1546	CD1	TYR A 366	28.234	14.421	53.313	1.00	27.40	C

-157-

	ATOM	1547	CD2	TYR	A	366	28.017	12.079	53.759	1.00	27.61	C
	ATOM	1548	CE1	TYR	A	366	28.912	14.144	52.130	1.00	28.23	C
	ATOM	1549	CE2	TYR	A	366	28.697	11.790	52.578	1.00	28.00	C
5	ATOM	1550	CZ	TYR	A	366	29.143	12.825	51.770	1.00	28.28	C
	ATOM	1551	OH	TYR	A	366	29.838	12.546	50.615	1.00	28.34	O
	ATOM	1552	N	ILE	A	367	28.692	16.310	56.174	1.00	30.76	N
	ATOM	1553	CA	ILE	A	367	29.559	17.412	55.762	1.00	32.74	C
	ATOM	1554	C	ILE	A	367	30.823	17.533	56.614	1.00	35.15	C
10	ATOM	1555	O	ILE	A	367	31.924	17.688	56.086	1.00	35.56	O
	ATOM	1556	CB	ILE	A	367	28.805	18.763	55.807	1.00	32.16	C
	ATOM	1557	CG1	ILE	A	367	27.685	18.764	54.763	1.00	32.04	C
	ATOM	1558	CG2	ILE	A	367	29.769	19.915	55.535	1.00	32.16	C
	ATOM	1559	CD1	ILE	A	367	26.790	19.977	54.829	1.00	32.66	C
15	ATOM	1560	N	ARG	A	368	30.660	17.465	57.930	1.00	38.07	N
	ATOM	1561	CA	ARG	A	368	31.794	17.582	58.842	1.00	41.56	C
	ATOM	1562	C	ARG	A	368	32.749	16.406	58.711	1.00	43.08	C
	ATOM	1563	O	ARG	A	368	33.963	16.558	58.845	1.00	43.32	O
	ATOM	1564	CB	ARG	A	368	31.309	17.652	60.289	1.00	43.01	C
20	ATOM	1565	CG	ARG	A	368	30.469	18.868	60.627	1.00	46.92	C
	ATOM	1566	CD	ARG	A	368	30.023	18.814	62.081	1.00	50.17	C
	ATOM	1567	NE	ARG	A	368	29.222	17.621	62.348	1.00	53.52	N
	ATOM	1568	CZ	ARG	A	368	28.703	17.315	63.531	1.00	54.12	C
	ATOM	1569	NH1	ARG	A	368	28.901	18.117	64.570	1.00	55.63	N
25	ATOM	1570	NH2	ARG	A	368	27.983	16.210	63.676	1.00	55.17	N
	ATOM	1571	N	CYS	A	369	32.187	15.234	58.440	1.00	44.44	N
	ATOM	1572	CA	CYS	A	369	32.964	14.011	58.333	1.00	46.85	C
	ATOM	1573	C	CYS	A	369	33.501	13.644	56.949	1.00	46.74	C
	ATOM	1574	O	CYS	A	369	34.641	13.198	56.828	1.00	46.26	O
30	ATOM	1575	CB	CYS	A	369	32.128	12.848	58.881	1.00	48.76	C
	ATOM	1576	SG	CYS	A	369	32.925	11.238	58.816	1.00	56.08	S
	ATOM	1577	N	ARG	A	370	32.700	13.841	55.905	1.00	47.07	N
	ATOM	1578	CA	ARG	A	370	33.123	13.457	54.558	1.00	47.21	C
	ATOM	1579	C	ARG	A	370	33.451	14.563	53.559	1.00	47.24	C
35	ATOM	1580	O	ARG	A	370	34.058	14.292	52.520	1.00	46.93	O
	ATOM	1581	CB	ARG	A	370	32.068	12.533	53.940	1.00	47.76	C
	ATOM	1582	CG	ARG	A	370	31.827	11.248	54.719	1.00	49.65	C
	ATOM	1583	CD	ARG	A	370	33.034	10.323	54.660	1.00	51.30	C
	ATOM	1584	NE	ARG	A	370	32.881	9.160	55.532	1.00	52.96	N
40	ATOM	1585	CZ	ARG	A	370	31.913	8.254	55.420	1.00	53.67	C
	ATOM	1586	NH1	ARG	A	370	30.999	8.367	54.465	1.00	54.23	N
	ATOM	1587	NH2	ARG	A	370	31.857	7.236	56.268	1.00	54.08	N
	ATOM	1588	N	HIS	A	371	33.059	15.799	53.845	1.00	46.83	N
	ATOM	1589	CA	HIS	A	371	33.340	16.879	52.908	1.00	47.01	C
45	ATOM	1590	C	HIS	A	371	34.670	17.554	53.217	1.00	47.99	C
	ATOM	1591	O	HIS	A	371	34.809	18.227	54.237	1.00	46.99	O
	ATOM	1592	CB	HIS	A	371	32.225	17.924	52.927	1.00	45.11	C
	ATOM	1593	CG	HIS	A	371	32.126	18.713	51.659	1.00	44.21	C
	ATOM	1594	ND1	HIS	A	371	31.086	18.559	50.768	1.00	43.28	N
50	ATOM	1595	CD2	HIS	A	371	32.959	19.629	51.111	1.00	43.81	C
	ATOM	1596	CE1	HIS	A	371	31.282	19.346	49.725	1.00	43.79	C
	ATOM	1597	NE2	HIS	A	371	32.412	20.005	49.907	1.00	43.86	N
	ATOM	1598	N	PRO	A	372	35.665	17.383	52.331	1.00	49.67	N
	ATOM	1599	CA	PRO	A	372	36.998	17.972	52.497	1.00	51.25	C
55	ATOM	1600	C	PRO	A	372	37.027	19.480	52.256	1.00	52.68	C
	ATOM	1601	O	PRO	A	372	36.223	20.013	51.489	1.00	52.39	O
	ATOM	1602	CB	PRO	A	372	37.833	17.208	51.476	1.00	51.31	C
	ATOM	1603	CG	PRO	A	372	36.853	16.991	50.366	1.00	51.05	C
	ATOM	1604	CD	PRO	A	372	35.613	16.549	51.115	1.00	50.21	C

-158-

	ATOM	1605	N	PRO A 373	37.961	20.187	52.914	1.00	54.03	N
	ATOM	1606	CA	PRO A 373	38.107	21.640	52.777	1.00	55.28	C
	ATOM	1607	C	PRO A 373	38.693	22.028	51.420	1.00	56.14	C
5	ATOM	1608	O	PRO A 373	39.284	21.197	50.731	1.00	56.44	O
	ATOM	1609	CB	PRO A 373	39.036	21.998	53.932	1.00	55.37	C
	ATOM	1610	CG	PRO A 373	39.925	20.793	54.011	1.00	55.24	C
	ATOM	1611	CD	PRO A 373	38.934	19.653	53.885	1.00	54.59	C
	ATOM	1612	N	PRO A 374	38.535	23.299	51.017	1.00	56.81	N
10	ATOM	1613	CA	PRO A 374	37.848	24.368	51.750	1.00	57.49	C
	ATOM	1614	C	PRO A 374	36.324	24.301	51.617	1.00	57.83	C
	ATOM	1615	O	PRO A 374	35.642	24.299	52.664	1.00	58.58	O
	ATOM	1616	CB	PRO A 374	38.431	25.631	51.127	1.00	57.24	C
	ATOM	1617	CG	PRO A 374	38.601	25.226	49.698	1.00	57.37	C
15	ATOM	1618	CD	PRO A 374	39.194	23.834	49.811	1.00	57.05	C
	ATOM	1619	N	LEU A 378	30.279	26.156	57.018	1.00	49.88	N
	ATOM	1620	CA	LEU A 378	29.679	27.221	56.220	1.00	45.66	C
	ATOM	1621	C	LEU A 378	28.825	26.586	55.127	1.00	41.60	C
	ATOM	1622	O	LEU A 378	27.802	27.138	54.723	1.00	38.14	O
20	ATOM	1623	CB	LEU A 378	30.769	28.092	55.590	1.00	53.84	C
	ATOM	1624	CG	LEU A 378	30.382	29.273	54.702	1.00	57.56	C
	ATOM	1625	CD1	LEU A 378	29.709	30.349	55.545	1.00	59.64	C
	ATOM	1626	CD2	LEU A 378	31.634	29.822	54.017	1.00	59.59	C
	ATOM	1627	N	LEU A 379	29.370	25.200	54.660	1.00	35.28	N
25	ATOM	1628	CA	LEU A 379	28.529	24.615	53.626	1.00	33.21	C
	ATOM	1629	C	LEU A 379	27.095	24.355	54.080	1.00	32.24	C
	ATOM	1630	O	LEU A 379	26.157	24.594	53.325	1.00	31.09	O
	ATOM	1631	CB	LEU A 379	29.151	23.309	53.121	1.00	33.21	C
	ATOM	1632	CG	LEU A 379	28.379	22.603	52.003	1.00	31.83	C
30	ATOM	1633	CD1	LEU A 379	28.301	23.508	50.783	1.00	33.04	C
	ATOM	1634	CD2	LEU A 379	29.066	21.292	51.651	1.00	32.12	C
	ATOM	1635	N	TYR A 380	26.917	23.869	55.304	1.00	31.72	N
	ATOM	1636	CA	TYR A 380	25.572	23.588	55.792	1.00	32.34	C
	ATOM	1637	C	TYR A 380	24.717	24.852	55.780	1.00	32.63	C
35	ATOM	1638	O	TYR A 380	23.562	24.833	55.339	1.00	31.56	O
	ATOM	1639	CB	TYR A 380	25.611	23.008	57.208	1.00	33.03	C
	ATOM	1640	CG	TYR A 380	24.239	22.659	57.743	1.00	34.66	C
	ATOM	1641	CD1	TYR A 380	23.486	21.635	57.169	1.00	35.98	C
	ATOM	1642	CD2	TYR A 380	23.680	23.373	58.800	1.00	35.42	C
40	ATOM	1643	CE1	TYR A 380	22.209	21.333	57.636	1.00	36.98	C
	ATOM	1644	CE2	TYR A 380	22.410	23.080	59.274	1.00	36.43	C
	ATOM	1645	CZ	TYR A 380	21.679	22.060	58.688	1.00	37.93	C
	ATOM	1646	OH	TYR A 380	20.420	21.770	59.154	1.00	38.77	O
	ATOM	1647	N	ALA A 381	25.288	25.950	56.266	1.00	32.03	N
45	ATOM	1648	CA	ALA A 381	24.578	27.223	56.304	1.00	32.04	C
	ATOM	1649	C	ALA A 381	24.190	27.683	54.902	1.00	31.59	C
	ATOM	1650	O	ALA A 381	23.084	28.187	54.693	1.00	32.20	O
	ATOM	1651	CB	ALA A 381	25.443	28.287	56.981	1.00	32.84	C
	ATOM	1652	N	LYS A 382	25.101	27.515	53.948	1.00	30.09	N
50	ATOM	1653	CA	LYS A 382	24.849	27.916	52.570	1.00	30.96	C
	ATOM	1654	C	LYS A 382	23.739	27.083	51.943	1.00	30.08	C
	ATOM	1655	O	LYS A 382	22.989	27.575	51.101	1.00	30.60	O
	ATOM	1656	CB	LYS A 382	26.121	27.781	51.731	1.00	31.98	C
	ATOM	1657	CG	LYS A 382	27.223	28.757	52.109	1.00	34.76	C
55	ATOM	1658	CD	LYS A 382	28.458	28.545	51.254	1.00	38.05	C
	ATOM	1659	CE	LYS A 382	29.559	29.526	51.615	1.00	39.31	C
	ATOM	1660	NZ	LYS A 382	30.806	29.245	50.845	1.00	41.47	N
	ATOM	1661	N	MET A 383	23.648	25.819	52.345	1.00	29.65	N
	ATOM	1662	CA	MET A 383	22.621	24.923	51.821	1.00	29.41	C

-159-

	ATOM	1663	C	MET A 383	21.253	25.286	52.389	1.00	29.82	C
	ATOM	1664	O	MET A 383	20.250	25.271	51.677	1.00	29.12	O
	ATOM	1665	CB	MET A 383	22.958	23.468	52.165	1.00	28.17	C
5	ATOM	1666	CG	MET A 383	24.130	22.908	51.381	1.00	28.12	C
	ATOM	1667	SD	MET A 383	24.510	21.186	51.776	1.00	28.48	S
	ATOM	1668	CE	MET A 383	23.099	20.338	51.048	1.00	28.89	C
	ATOM	1669	N	ILE A 384	21.215	25.612	53.676	1.00	30.76	N
	ATOM	1670	CA	ILE A 384	19.960	25.983	54.319	1.00	32.84	C
10	ATOM	1671	C	ILE A 384	19.422	27.271	53.701	1.00	32.96	C
	ATOM	1672	O	ILE A 384	18.208	27.458	53.594	1.00	32.83	O
	ATOM	1673	CB	ILE A 384	20.149	26.186	55.842	1.00	34.53	C
	ATOM	1674	CG1	ILE A 384	20.651	24.889	56.482	1.00	36.66	C
	ATOM	1675	CG2	ILE A 384	18.834	26.610	56.482	1.00	36.24	C
15	ATOM	1676	CD1	ILE A 384	19.744	23.691	56.257	1.00	37.66	C
	ATOM	1677	N	GLN A 385	20.328	28.153	53.287	1.00	32.82	N
	ATOM	1678	CA	GLN A 385	19.931	29.412	52.669	1.00	33.03	C
	ATOM	1679	C	GLN A 385	19.288	29.174	51.303	1.00	32.26	C
	ATOM	1680	O	GLN A 385	18.382	29.905	50.901	1.00	30.38	O
20	ATOM	1681	CB	GLN A 385	21.136	30.342	52.515	1.00	35.19	C
	ATOM	1682	CG	GLN A 385	20.839	31.588	51.692	1.00	39.54	C
	ATOM	1683	CD	GLN A 385	19.705	32.421	52.270	1.00	41.95	C
	ATOM	1684	OE1	GLN A 385	19.024	33.151	51.545	1.00	44.07	O
	ATOM	1685	NE2	GLN A 385	19.504	32.324	53.579	1.00	42.90	N
25	ATOM	1686	N	LYS A 386	19.756	28.152	50.591	1.00	30.96	N
	ATOM	1687	CA	LYS A 386	19.197	27.840	49.282	1.00	30.88	C
	ATOM	1688	C	LYS A 386	17.748	27.415	49.447	1.00	29.98	C
	ATOM	1689	O	LYS A 386	16.927	27.635	48.558	1.00	29.72	O
	ATOM	1690	CB	LYS A 386	19.985	26.719	48.601	1.00	32.29	C
30	ATOM	1691	CG	LYS A 386	21.430	27.064	48.310	1.00	35.09	C
	ATOM	1692	CD	LYS A 386	21.539	28.305	47.453	1.00	36.92	C
	ATOM	1693	CE	LYS A 386	22.997	28.643	47.170	1.00	39.17	C
	ATOM	1694	NZ	LYS A 386	23.133	30.008	46.589	1.00	40.63	N
	ATOM	1695	N	LEU A 387	17.433	26.804	50.583	1.00	29.25	N
35	ATOM	1696	CA	LEU A 387	16.064	26.373	50.833	1.00	29.50	C
	ATOM	1697	C	LEU A 387	15.172	27.604	50.982	1.00	29.30	C
	ATOM	1698	O	LEU A 387	14.014	27.594	50.572	1.00	27.98	O
	ATOM	1699	CB	LEU A 387	15.988	25.503	52.091	1.00	30.49	C
	ATOM	1700	CG	LEU A 387	16.625	24.111	51.980	1.00	31.01	C
40	ATOM	1701	CD1	LEU A 387	16.443	23.363	53.289	1.00	33.01	C
	ATOM	1702	CD2	LEU A 387	15.985	23.339	50.839	1.00	31.27	C
	ATOM	1703	N	ALA A 388	15.714	28.667	51.566	1.00	28.72	N
	ATOM	1704	CA	ALA A 388	14.952	29.903	51.735	1.00	29.54	C
	ATOM	1705	C	ALA A 388	14.757	30.557	50.367	1.00	29.67	C
45	ATOM	1706	O	ALA A 388	13.696	31.121	50.082	1.00	29.63	O
	ATOM	1707	CB	ALA A 388	15.687	30.856	52.679	1.00	30.01	C
	ATOM	1708	N	ASP A 389	15.786	30.479	49.524	1.00	29.62	N
	ATOM	1709	CA	ASP A 389	15.730	31.044	48.175	1.00	30.08	C
	ATOM	1710	C	ASP A 389	14.625	30.360	47.378	1.00	29.78	C
50	ATOM	1711	O	ASP A 389	13.917	31.000	46.598	1.00	29.18	O
	ATOM	1712	CB	ASP A 389	17.059	30.833	47.445	1.00	31.12	C
	ATOM	1713	CG	ASP A 389	18.183	31.682	48.006	1.00	34.91	C
	ATOM	1714	OD1	ASP A 389	19.352	31.423	47.643	1.00	36.63	O
	ATOM	1715	OD2	ASP A 389	17.901	32.608	48.796	1.00	35.52	O
55	ATOM	1716	N	LEU A 390	14.496	29.052	47.572	1.00	27.64	N
	ATOM	1717	CA	LEU A 390	13.482	28.262	46.881	1.00	28.50	C
	ATOM	1718	C	LEU A 390	12.067	28.730	47.223	1.00	27.80	C
	ATOM	1719	O	LEU A 390	11.187	28.740	46.360	1.00	26.98	O
	ATOM	1720	CB	LEU A 390	13.646	26.786	47.252	1.00	28.87	C

-160-

	ATOM	1721	CG	LEU A 390	14.130	25.761	46.221	1.00	31.08	C
	ATOM	1722	CD1	LEU A 390	14.754	26.424	45.017	1.00	31.00	C
	ATOM	1723	CD2	LEU A 390	15.101	24.810	46.902	1.00	31.75	C
5	ATOM	1724	N	ARG A 391	11.849	29.109	48.481	1.00	27.87	N
	ATOM	1725	CA	ARG A 391	10.535	29.574	48.917	1.00	28.52	C
	ATOM	1726	C	ARG A 391	10.132	30.808	48.125	1.00	28.78	C
	ATOM	1727	O	ARG A 391	8.968	30.961	47.757	1.00	28.82	O
	ATOM	1728	CB	ARG A 391	10.536	29.919	50.415	1.00	30.35	C
10	ATOM	1729	CG	ARG A 391	10.795	28.744	51.354	1.00	32.51	C
	ATOM	1730	CD	ARG A 391	9.743	27.658	51.208	1.00	34.99	C
	ATOM	1731	NE	ARG A 391	9.952	26.552	52.141	1.00	37.12	N
	ATOM	1732	CZ	ARG A 391	9.395	26.460	53.346	1.00	37.91	C
	ATOM	1733	NH1	ARG A 391	8.580	27.411	53.783	1.00	38.94	N
	ATOM	1734	NH2	ARG A 391	9.646	25.408	54.115	1.00	37.42	N
15	ATOM	1735	N	SER A 392	11.094	31.690	47.865	1.00	28.76	N
	ATOM	1736	CA	SER A 392	10.811	32.908	47.114	1.00	29.36	C
	ATOM	1737	C	SER A 392	10.483	32.588	45.664	1.00	28.02	C
	ATOM	1738	O	SER A 392	9.577	33.178	45.082	1.00	28.38	O
	ATOM	1739	CB	SER A 392	11.997	33.866	47.185	1.00	31.21	C
20	ATOM	1740	OG	SER A 392	12.192	34.305	48.518	1.00	37.19	O
	ATOM	1741	N	LEU A 393	11.219	31.648	45.081	1.00	26.23	N
	ATOM	1742	CA	LEU A 393	10.972	31.253	43.700	1.00	26.10	C
	ATOM	1743	C	LEU A 393	9.614	30.567	43.586	1.00	25.57	C
	ATOM	1744	O	LEU A 393	8.919	30.705	42.576	1.00	26.87	O
25	ATOM	1745	CB	LEU A 393	12.081	30.309	43.216	1.00	26.02	C
	ATOM	1746	CG	LEU A 393	13.450	30.968	43.030	1.00	26.66	C
	ATOM	1747	CD1	LEU A 393	14.536	29.905	42.878	1.00	28.52	C
	ATOM	1748	CD2	LEU A 393	13.400	31.869	41.808	1.00	29.45	C
	ATOM	1749	N	ASN A 394	9.242	29.825	44.625	1.00	24.50	N
30	ATOM	1750	CA	ASN A 394	7.964	29.122	44.656	1.00	26.07	C
	ATOM	1751	C	ASN A 394	6.855	30.167	44.570	1.00	27.28	C
	ATOM	1752	O	ASN A 394	5.929	30.055	43.764	1.00	26.29	O
	ATOM	1753	CB	ASN A 394	7.827	28.347	45.967	1.00	26.75	C
	ATOM	1754	CG	ASN A 394	6.646	27.397	45.968	1.00	28.26	C
35	ATOM	1755	OD1	ASN A 394	5.660	27.604	45.263	1.00	28.24	O
	ATOM	1756	ND2	ASN A 394	6.736	26.352	46.779	1.00	28.79	N
	ATOM	1757	N	GLU A 395	6.966	31.188	45.413	1.00	28.62	N
	ATOM	1758	CA	GLU A 395	5.986	32.266	45.464	1.00	30.55	C
	ATOM	1759	C	GLU A 395	5.815	32.976	44.130	1.00	29.66	C
40	ATOM	1760	O	GLU A 395	4.691	33.213	43.684	1.00	29.50	O
	ATOM	1761	CB	GLU A 395	6.385	33.280	46.536	1.00	33.44	C
	ATOM	1762	CG	GLU A 395	6.277	32.744	47.954	1.00	40.01	C
	ATOM	1763	CD	GLU A 395	4.838	32.481	48.366	1.00	44.38	C
	ATOM	1764	OE1	GLU A 395	4.618	32.045	49.518	1.00	46.89	O
45	ATOM	1765	OE2	GLU A 395	3.924	32.713	47.540	1.00	46.99	O
	ATOM	1766	N	GLU A 396	6.929	33.324	43.496	1.00	29.08	N
	ATOM	1767	CA	GLU A 396	6.871	34.013	42.217	1.00	28.78	C
	ATOM	1768	C	GLU A 396	6.280	33.102	41.148	1.00	28.20	C
	ATOM	1769	O	GLU A 396	5.486	33.545	40.317	1.00	27.96	O
50	ATOM	1770	CB	GLU A 396	8.265	34.490	41.791	1.00	30.45	C
	ATOM	1771	CG	GLU A 396	8.276	35.254	40.465	1.00	30.29	C
	ATOM	1772	CD	GLU A 396	7.502	36.568	40.525	1.00	33.32	C
	ATOM	1773	OE1	GLU A 396	7.098	37.068	39.452	1.00	32.46	O
	ATOM	1774	OE2	GLU A 396	7.307	37.108	41.639	1.00	32.27	O
55	ATOM	1775	N	HIS A 397	6.651	31.826	41.162	1.00	26.94	N
	ATOM	1776	CA	HIS A 397	6.104	30.919	40.162	1.00	27.05	C
	ATOM	1777	C	HIS A 397	4.583	30.835	40.295	1.00	27.50	C
	ATOM	1778	O	HIS A 397	3.866	30.834	39.294	1.00	27.05	O

-161-

	ATOM	1779	CB	HIS	A	397	6.718	29.519	40.282	1.00	26.64	C
	ATOM	1780	CG	HIS	A	397	6.058	28.507	39.400	1.00	26.04	C
	ATOM	1781	ND1	HIS	A	397	4.999	27.731	39.822	1.00	27.22	N
5	ATOM	1782	CD2	HIS	A	397	6.227	28.228	38.086	1.00	26.36	C
	ATOM	1783	CE1	HIS	A	397	4.542	27.024	38.805	1.00	26.59	C
	ATOM	1784	NE2	HIS	A	397	5.268	27.308	37.740	1.00	26.30	N
	ATOM	1785	N	SER	A	398	4.094	30.785	41.529	1.00	28.04	N
	ATOM	1786	CA	SER	A	398	2.657	30.696	41.775	1.00	29.62	C
10	ATOM	1787	C	SER	A	398	1.921	31.901	41.195	1.00	29.87	C
	ATOM	1788	O	SER	A	398	0.862	31.761	40.579	1.00	28.32	O
	ATOM	1789	CB	SER	A	398	2.389	30.604	43.279	1.00	31.44	C
	ATOM	1790	OG	SER	A	398	1.000	30.483	43.534	1.00	38.72	O
	ATOM	1791	N	LYS	A	399	2.485	33.085	41.397	1.00	30.06	N
15	ATOM	1792	CA	LYS	A	399	1.882	34.313	40.885	1.00	31.61	C
	ATOM	1793	C	LYS	A	399	1.807	34.283	39.363	1.00	30.91	C
	ATOM	1794	O	LYS	A	399	0.790	34.651	38.771	1.00	30.21	O
	ATOM	1795	CB	LYS	A	399	2.698	35.527	41.336	1.00	33.79	C
	ATOM	1796	CG	LYS	A	399	2.754	35.693	42.842	1.00	38.63	C
20	ATOM	1797	CD	LYS	A	399	3.521	36.946	43.236	1.00	41.48	C
	ATOM	1798	CE	LYS	A	399	3.571	37.101	44.750	1.00	43.57	C
	ATOM	1799	NZ	LYS	A	399	4.340	38.313	45.155	1.00	44.90	N
	ATOM	1800	N	GLN	A	400	2.886	33.834	38.731	1.00	29.20	N
	ATOM	1801	CA	GLN	A	400	2.926	33.770	37.278	1.00	28.78	C
25	ATOM	1802	C	GLN	A	400	2.052	32.660	36.702	1.00	27.95	C
	ATOM	1803	O	GLN	A	400	1.524	32.789	35.595	1.00	27.64	O
	ATOM	1804	CB	GLN	A	400	4.374	33.637	36.802	1.00	28.49	C
	ATOM	1805	CG	GLN	A	400	5.147	34.942	36.964	1.00	30.64	C
	ATOM	1806	CD	GLN	A	400	6.483	34.940	36.256	1.00	31.34	C
30	ATOM	1807	OE1	GLN	A	400	6.673	34.235	35.265	1.00	33.90	O
	ATOM	1808	NE2	GLN	A	400	7.414	35.751	36.749	1.00	31.02	N
	ATOM	1809	N	TYR	A	401	1.894	31.571	37.446	1.00	26.56	N
	ATOM	1810	CA	TYR	A	401	1.051	30.481	36.980	1.00	27.31	C
	ATOM	1811	C	TYR	A	401	-0.382	30.998	36.941	1.00	27.98	C
35	ATOM	1812	O	TYR	A	401	-1.147	30.686	36.024	1.00	27.25	O
	ATOM	1813	CB	TYR	A	401	1.127	29.285	37.931	1.00	27.75	C
	ATOM	1814	CG	TYR	A	401	0.229	28.147	37.516	1.00	27.44	C
	ATOM	1815	CD1	TYR	A	401	0.600	27.281	36.489	1.00	28.38	C
	ATOM	1816	CD2	TYR	A	401	-1.013	27.960	38.119	1.00	29.26	C
40	ATOM	1817	CE1	TYR	A	401	-0.242	26.260	36.068	1.00	28.43	C
	ATOM	1818	CE2	TYR	A	401	-1.868	26.938	37.703	1.00	29.62	C
	ATOM	1819	CZ	TYR	A	401	-1.475	26.094	36.677	1.00	29.95	C
	ATOM	1820	OH	TYR	A	401	-2.319	25.089	36.252	1.00	30.37	O
	ATOM	1821	N	ARG	A	402	-0.742	31.790	37.948	1.00	29.27	N
45	ATOM	1822	CA	ARG	A	402	-2.083	32.360	38.021	1.00	32.16	C
	ATOM	1823	C	ARG	A	402	-2.386	33.173	36.769	1.00	32.00	C
	ATOM	1824	O	ARG	A	402	-3.434	32.998	36.150	1.00	31.31	O
	ATOM	1825	CB	ARG	A	402	-2.220	33.251	39.256	1.00	36.10	C
	ATOM	1826	CG	ARG	A	402	-3.587	33.906	39.391	1.00	41.28	C
50	ATOM	1827	CD	ARG	A	402	-3.710	34.730	40.669	1.00	45.66	C
	ATOM	1828	NE	ARG	A	402	-3.552	33.916	41.873	1.00	49.74	N
	ATOM	1829	CZ	ARG	A	402	-2.382	33.582	42.410	1.00	51.64	C
	ATOM	1830	NH1	ARG	A	402	-1.249	33.996	41.856	1.00	52.67	N
	ATOM	1831	NH2	ARG	A	402	-2.343	32.825	43.499	1.00	52.69	N
55	ATOM	1832	N	CYS	A	403	-1.471	34.066	36.402	1.00	32.10	N
	ATOM	1833	CA	CYS	A	403	-1.645	34.895	35.210	1.00	33.04	C
	ATOM	1834	C	CYS	A	403	-1.781	34.014	33.976	1.00	32.14	C
	ATOM	1835	O	CYS	A	403	-2.620	34.257	33.106	1.00	30.55	O
	ATOM	1836	CB	CYS	A	403	-0.450	35.838	35.030	1.00	35.60	C

-162-

	ATOM	1837	SG	CYS A 403	-0.253	36.492	33.340	1.00	44.46	S
	ATOM	1838	N	LEU A 404	-0.950	32.980	33.911	1.00	30.59	N
	ATOM	1839	CA	LEU A 404	-0.967	32.065	32.784	1.00	30.86	C
5	ATOM	1840	C	LEU A 404	-2.327	31.390	32.638	1.00	29.62	C
	ATOM	1841	O	LEU A 404	-2.840	31.256	31.529	1.00	30.21	O
	ATOM	1842	CB	LEU A 404	0.130	31.008	32.955	1.00	32.55	C
	ATOM	1843	CG	LEU A 404	0.353	30.078	31.766	1.00	34.87	C
	ATOM	1844	CD1	LEU A 404	0.840	30.895	30.580	1.00	36.26	C
10	ATOM	1845	CD2	LEU A 404	1.370	29.005	32.127	1.00	35.52	C
	ATOM	1846	N	SER A 405	-2.918	30.987	33.760	1.00	29.30	N
	ATOM	1847	CA	SER A 405	-4.212	30.309	33.749	1.00	29.83	C
	ATOM	1848	C	SER A 405	-5.358	31.173	33.218	1.00	28.16	C
	ATOM	1849	O	SER A 405	-6.423	30.651	32.885	1.00	28.54	O
15	ATOM	1850	CB	SER A 405	-4.563	29.802	35.153	1.00	31.58	C
	ATOM	1851	OG	SER A 405	-4.841	30.873	36.040	1.00	34.11	O
	ATOM	1852	N	PHE A 406	-5.147	32.484	33.145	1.00	25.99	N
	ATOM	1853	CA	PHE A 406	-6.179	33.396	32.636	1.00	26.56	C
	ATOM	1854	C	PHE A 406	-6.263	33.340	31.112	1.00	26.23	C
20	ATOM	1855	O	PHE A 406	-7.256	33.778	30.518	1.00	25.59	O
	ATOM	1856	CB	PHE A 406	-5.868	34.842	33.042	1.00	26.14	C
	ATOM	1857	CG	PHE A 406	-6.058	35.128	34.503	1.00	28.26	C
	ATOM	1858	CD1	PHE A 406	-5.386	36.196	35.099	1.00	29.88	C
	ATOM	1859	CD2	PHE A 406	-6.920	34.361	35.278	1.00	29.84	C
25	ATOM	1860	CE1	PHE A 406	-5.570	36.494	36.446	1.00	30.77	C
	ATOM	1861	CE2	PHE A 406	-7.112	34.651	36.632	1.00	31.26	C
	ATOM	1862	CZ	PHE A 406	-6.436	35.719	37.214	1.00	30.45	C
	ATOM	1863	N	GLN A 407	-5.220	32.814	30.478	1.00	25.64	N
	ATOM	1864	CA	GLN A 407	-5.189	32.748	29.019	1.00	25.17	C
30	ATOM	1865	C	GLN A 407	-6.155	31.687	28.500	1.00	25.33	C
	ATOM	1866	O	GLN A 407	-6.086	30.524	28.903	1.00	24.86	O
	ATOM	1867	CB	GLN A 407	-3.765	32.448	28.527	1.00	25.99	C
	ATOM	1868	CG	GLN A 407	-3.571	32.694	27.030	1.00	26.23	C
	ATOM	1869	CD	GLN A 407	-3.718	34.165	26.651	1.00	26.81	C
35	ATOM	1870	OE1	GLN A 407	-4.087	34.494	25.520	1.00	28.94	O
	ATOM	1871	NE2	GLN A 407	-3.414	35.052	27.590	1.00	21.63	N
	ATOM	1872	N	PRO A 408	-7.083	32.079	27.608	1.00	25.83	N
	ATOM	1873	CA	PRO A 408	-8.052	31.124	27.058	1.00	27.42	C
	ATOM	1874	C	PRO A 408	-7.384	29.913	26.398	1.00	29.12	C
40	ATOM	1875	O	PRO A 408	-6.389	30.056	25.688	1.00	29.12	O
	ATOM	1876	CB	PRO A 408	-8.835	31.967	26.054	1.00	25.96	C
	ATOM	1877	CG	PRO A 408	-8.824	33.331	26.690	1.00	25.60	C
	ATOM	1878	CD	PRO A 408	-7.376	33.449	27.142	1.00	26.30	C
	ATOM	1879	N	GLU A 409	-7.941	28.731	26.646	1.00	31.66	N
45	ATOM	1880	CA	GLU A 409	-7.441	27.479	26.078	1.00	34.64	C
	ATOM	1881	C	GLU A 409	-6.104	27.014	26.661	1.00	34.56	C
	ATOM	1882	O	GLU A 409	-5.480	26.100	26.122	1.00	34.24	O
	ATOM	1883	CB	GLU A 409	-7.293	27.606	24.555	1.00	37.88	C
	ATOM	1884	CG	GLU A 409	-8.511	28.167	23.823	1.00	43.65	C
50	ATOM	1885	CD	GLU A 409	-9.724	27.259	23.887	1.00	46.69	C
	ATOM	1886	OE1	GLU A 409	-10.252	27.039	24.998	1.00	49.95	O
	ATOM	1887	OE2	GLU A 409	-10.153	26.766	22.821	1.00	49.48	O
	ATOM	1888	N	CYS A 410	-5.671	27.628	27.759	1.00	33.81	N
	ATOM	1889	CA	CYS A 410	-4.399	27.267	28.382	1.00	35.08	C
55	ATOM	1890	C	CYS A 410	-4.396	25.871	29.002	1.00	34.78	C
	ATOM	1891	O	CYS A 410	-3.390	25.164	28.943	1.00	34.24	O
	ATOM	1892	CB	CYS A 410	-4.027	28.299	29.455	1.00	36.13	C
	ATOM	1893	SG	CYS A 410	-2.433	28.006	30.271	1.00	41.53	S
	ATOM	1894	N	SER A 411	-5.518	25.472	29.593	1.00	34.62	N

-163-

	ATOM	1895	CA	SER A 411	-5.611	24.163	30.235	1.00	35.60	C
	ATOM	1896	C	SER A 411	-5.215	23.008	29.319	1.00	35.51	C
	ATOM	1897	O	SER A 411	-4.602	22.040	29.770	1.00	35.62	O
5	ATOM	1898	CB	SER A 411	-7.031	23.928	30.763	1.00	36.58	C
	ATOM	1899	OG	SER A 411	-7.959	23.837	29.697	1.00	38.87	O
	ATOM	1900	N	MET A 412	-5.561	23.108	28.038	1.00	35.70	N
	ATOM	1901	CA	MET A 412	-5.244	22.053	27.079	1.00	36.25	C
	ATOM	1902	C	MET A 412	-3.744	21.912	26.846	1.00	34.53	C
10	ATOM	1903	O	MET A 412	-3.273	20.867	26.393	1.00	34.48	O
	ATOM	1904	CB	MET A 412	-5.936	22.324	25.741	1.00	40.58	C
	ATOM	1905	CG	MET A 412	-7.433	22.563	25.850	1.00	45.64	C
	ATOM	1906	SD	MET A 412	-8.214	22.729	24.232	1.00	52.62	S
	ATOM	1907	CE	MET A 412	-7.402	24.204	23.610	1.00	50.53	C
15	ATOM	1908	N	LYS A 413	-2.996	22.965	27.150	1.00	31.53	N
	ATOM	1909	CA	LYS A 413	-1.551	22.944	26.960	1.00	30.85	C
	ATOM	1910	C	LYS A 413	-0.831	22.407	28.192	1.00	30.52	C
	ATOM	1911	O	LYS A 413	0.386	22.236	28.187	1.00	30.68	O
	ATOM	1912	CB	LYS A 413	-1.042	24.350	26.632	1.00	31.05	C
20	ATOM	1913	CG	LYS A 413	-1.557	24.897	25.307	1.00	32.36	C
	ATOM	1914	CD	LYS A 413	-1.030	26.296	25.035	1.00	32.77	C
	ATOM	1915	CE	LYS A 413	-1.521	26.812	23.689	1.00	34.50	C
	ATOM	1916	NZ	LYS A 413	-3.014	26.878	23.622	1.00	36.17	N
	ATOM	1917	N	LEU A 414	-1.590	22.142	29.248	1.00	30.09	N
25	ATOM	1918	CA	LEU A 414	-1.014	21.620	30.484	1.00	28.96	C
	ATOM	1919	C	LEU A 414	-1.393	20.147	30.610	1.00	28.33	C
	ATOM	1920	O	LEU A 414	-1.654	19.489	29.604	1.00	29.10	O
	ATOM	1921	CB	LEU A 414	-1.544	22.427	31.676	1.00	28.64	C
	ATOM	1922	CG	LEU A 414	-1.270	23.934	31.581	1.00	30.41	C
30	ATOM	1923	CD1	LEU A 414	-1.967	24.676	32.711	1.00	31.19	C
	ATOM	1924	CD2	LEU A 414	0.226	24.179	31.624	1.00	30.79	C
	ATOM	1925	N	THR A 415	-1.401	19.624	31.833	1.00	27.70	N
	ATOM	1926	CA	THR A 415	-1.779	18.232	32.071	1.00	26.69	C
	ATOM	1927	C	THR A 415	-2.620	18.195	33.338	1.00	26.91	C
35	ATOM	1928	O	THR A 415	-2.548	19.104	34.157	1.00	26.39	O
	ATOM	1929	CB	THR A 415	-0.556	17.310	32.307	1.00	26.61	C
	ATOM	1930	OG1	THR A 415	-0.006	17.570	33.607	1.00	25.35	O
	ATOM	1931	CG2	THR A 415	0.509	17.546	31.247	1.00	26.48	C
	ATOM	1932	N	PRO A 416	-3.432	17.142	33.516	1.00	27.60	N
40	ATOM	1933	CA	PRO A 416	-4.269	17.037	34.717	1.00	27.16	C
	ATOM	1934	C	PRO A 416	-3.477	17.169	36.026	1.00	27.48	C
	ATOM	1935	O	PRO A 416	-3.930	17.813	36.975	1.00	26.90	O
	ATOM	1936	CB	PRO A 416	-4.908	15.661	34.564	1.00	29.00	C
	ATOM	1937	CG	PRO A 416	-5.083	15.555	33.072	1.00	28.36	C
45	ATOM	1938	CD	PRO A 416	-3.752	16.071	32.553	1.00	28.22	C
	ATOM	1939	N	LEU A 417	-2.294	16.560	36.072	1.00	25.90	N
	ATOM	1940	CA	LEU A 417	-1.460	16.610	37.271	1.00	25.39	C
	ATOM	1941	C	LEU A 417	-0.961	18.031	37.545	1.00	24.67	C
	ATOM	1942	O	LEU A 417	-0.983	18.502	38.685	1.00	24.55	O
50	ATOM	1943	CB	LEU A 417	-0.279	15.643	37.124	1.00	25.12	C
	ATOM	1944	CG	LEU A 417	0.722	15.507	38.273	1.00	25.26	C
	ATOM	1945	CD1	LEU A 417	0.021	15.098	39.564	1.00	24.40	C
	ATOM	1946	CD2	LEU A 417	1.766	14.470	37.882	1.00	25.23	C
	ATOM	1947	N	VAL A 418	-0.506	18.711	36.500	1.00	24.66	N
55	ATOM	1948	CA	VAL A 418	-0.027	20.080	36.640	1.00	25.57	C
	ATOM	1949	C	VAL A 418	-1.176	20.971	37.111	1.00	26.33	C
	ATOM	1950	O	VAL A 418	-1.001	21.814	37.991	1.00	27.09	O
	ATOM	1951	CB	VAL A 418	0.531	20.599	35.297	1.00	25.14	C
	ATOM	1952	CG1	VAL A 418	0.723	22.112	35.338	1.00	26.89	C

-164-

	ATOM	1953	CG2	VAL	A	418	1.861	19.912	35.009	1.00	25.97	C
	ATOM	1954	N	LEU	A	419	-2.354	20.769	36.530	1.00	26.33	N
	ATOM	1955	CA	LEU	A	419	-3.526	21.556	36.902	1.00	27.78	C
5	ATOM	1956	C	LEU	A	419	-3.861	21.399	38.382	1.00	29.03	C
	ATOM	1957	O	LEU	A	419	-4.206	22.370	39.052	1.00	30.30	O
	ATOM	1958	CB	LEU	A	419	-4.733	21.143	36.051	1.00	28.60	C
	ATOM	1959	CG	LEU	A	419	-4.696	21.585	34.586	1.00	30.69	C
	ATOM	1960	CD1	LEU	A	419	-5.871	20.975	33.828	1.00	30.94	C
10	ATOM	1961	CD2	LEU	A	419	-4.743	23.105	34.515	1.00	31.11	C
	ATOM	1962	N	GLU	A	420	-3.738	20.184	38.904	1.00	29.76	N
	ATOM	1963	CA	GLU	A	420	-4.056	19.962	40.307	1.00	31.06	C
	ATOM	1964	C	GLU	A	420	-3.010	20.514	41.268	1.00	30.59	C
	ATOM	1965	O	GLU	A	420	-3.344	21.184	42.245	1.00	30.30	O
15	ATOM	1966	CB	GLU	A	420	-4.237	18.478	40.605	1.00	32.62	C
	ATOM	1967	CG	GLU	A	420	-4.697	18.251	42.037	1.00	36.69	C
	ATOM	1968	CD	GLU	A	420	-4.267	16.919	42.598	1.00	38.47	C
	ATOM	1969	OE1	GLU	A	420	-4.631	16.624	43.756	1.00	40.46	O
	ATOM	1970	OE2	GLU	A	420	-3.561	16.171	41.891	1.00	41.56	O
20	ATOM	1971	N	VAL	A	421	-1.744	20.223	40.992	1.00	31.25	N
	ATOM	1972	CA	VAL	A	421	-0.663	20.675	41.855	1.00	32.00	C
	ATOM	1973	C	VAL	A	421	-0.544	22.191	41.960	1.00	32.63	C
	ATOM	1974	O	VAL	A	421	-0.355	22.724	43.051	1.00	32.82	O
	ATOM	1975	CB	VAL	A	421	0.694	20.082	41.395	1.00	31.60	C
25	ATOM	1976	CG1	VAL	A	421	1.843	20.676	42.208	1.00	31.31	C
	ATOM	1977	CG2	VAL	A	421	0.667	18.567	41.556	1.00	31.20	C
	ATOM	1978	N	PHE	A	422	-0.670	22.890	40.839	1.00	33.47	N
	ATOM	1979	CA	PHE	A	422	-0.541	24.342	40.857	1.00	34.95	C
	ATOM	1980	C	PHE	A	422	-1.866	25.089	40.872	1.00	35.99	C
30	ATOM	1981	O	PHE	A	422	-1.907	26.284	41.159	1.00	36.37	O
	ATOM	1982	CB	PHE	A	422	0.310	24.794	39.670	1.00	34.60	C
	ATOM	1983	CG	PHE	A	422	1.679	24.182	39.656	1.00	34.76	C
	ATOM	1984	CD1	PHE	A	422	2.093	23.389	38.592	1.00	34.88	C
	ATOM	1985	CD2	PHE	A	422	2.545	24.369	40.728	1.00	35.16	C
35	ATOM	1986	CE1	PHE	A	422	3.348	22.790	38.597	1.00	34.92	C
	ATOM	1987	CE2	PHE	A	422	3.801	23.774	40.743	1.00	34.70	C
	ATOM	1988	CZ	PHE	A	422	4.202	22.982	39.674	1.00	34.73	C
	ATOM	1989	N	GLY	A	423	-2.946	24.378	40.570	1.00	37.39	N
	ATOM	1990	CA	GLY	A	423	-4.261	24.993	40.564	1.00	38.89	C
40	ATOM	1991	C	GLY	A	423	-4.914	24.907	41.930	1.00	39.70	C
	ATOM	1992	O	GLY	A	423	-5.857	24.099	42.083	1.00	40.52	O
	TER	1993		GLY	A	423						
	HETATM	1994	O2	VDX		425	17.029	18.071	34.819	1.00	21.73	O
	HETATM	1995	O3	VDX		425	4.489	26.946	35.054	1.00	24.67	O
45	HETATM	1996	C1	VDX		425	14.139	17.953	35.755	1.00	20.80	C
	HETATM	1997	C2	VDX		425	14.879	16.893	34.895	1.00	21.02	C
	HETATM	1998	C3	VDX		425	15.992	17.534	33.962	1.00	21.41	C
	HETATM	1999	C4	VDX		425	15.368	18.672	33.049	1.00	21.29	C
	HETATM	2000	C5	VDX		425	14.622	19.724	33.864	1.00	21.00	C
50	HETATM	2001	C6	VDX		425	14.797	21.120	33.792	1.00	20.95	C
	HETATM	2002	C7	VDX		425	14.174	22.286	34.514	1.00	21.23	C
	HETATM	2003	C8	VDX		425	13.966	23.488	34.042	1.00	21.54	C
	HETATM	2004	C9	VDX		425	14.354	23.927	32.544	1.00	21.77	C
	HETATM	2005	C10	VDX		425	13.602	19.075	34.828	1.00	20.74	C
55	HETATM	2006	C11	VDX		425	13.088	24.490	31.671	1.00	21.66	C
	HETATM	2007	C12	VDX		425	12.147	25.443	32.564	1.00	22.04	C
	HETATM	2008	C13	VDX		425	11.753	24.897	34.070	1.00	22.01	C
	HETATM	2009	C14	VDX		425	13.148	24.538	34.777	1.00	21.80	C
	HETATM	2010	C15	VDX		425	12.661	24.266	36.350	1.00	22.22	C

-165-

	HETATM	2011	C16	VDX	425	11.429	25.231	36.497	1.00	22.39	C
	HETATM	2012	C17	VDX	425	11.276	25.934	35.106	1.00	22.31	C
	HETATM	2013	C18	VDX	425	10.769	23.570	33.779	1.00	21.50	C
5	HETATM	2014	C19	VDX	425	12.291	19.455	34.852	1.00	20.77	C
	HETATM	2015	C20	VDX	425	9.849	26.546	34.726	1.00	22.90	C
	HETATM	2016	C21	VDX	425	9.804	27.956	35.482	1.00	23.65	C
	HETATM	2017	C22	VDX	425	8.575	25.824	35.268	1.00	23.16	C
	HETATM	2018	C23	VDX	425	7.331	26.060	34.405	1.00	23.73	C
10	HETATM	2019	C24	VDX	425	6.152	25.266	34.672	1.00	24.36	C
	HETATM	2020	C25	VDX	425	4.775	25.776	34.336	1.00	24.75	C
	HETATM	2021	C26	VDX	425	4.701	26.010	32.842	1.00	25.41	C
	HETATM	2022	C27	VDX	425	3.668	24.730	34.723	1.00	25.39	C
	HETATM	2023	O1	VDX	425	13.119	17.359	36.620	1.00	20.68	O
15	HETATM	2024	O	HOH	500	14.347	10.333	30.796	1.00	24.33	O
	HETATM	2025	O	HOH	501	13.828	12.782	35.922	1.00	21.46	O
	HETATM	2026	O	HOH	502	13.846	14.468	42.856	1.00	24.78	O
	HETATM	2027	O	HOH	503	19.132	15.890	40.266	1.00	21.27	O
	HETATM	2028	O	HOH	504	15.013	12.029	41.977	1.00	22.69	O
20	HETATM	2029	O	HOH	505	13.766	10.118	35.125	1.00	20.29	O
	HETATM	2030	O	HOH	506	16.290	13.157	34.345	1.00	30.57	O
	HETATM	2031	O	HOH	507	5.938	22.747	23.179	1.00	24.25	O
	HETATM	2032	O	HOH	508	13.771	7.592	35.963	1.00	28.23	O
	HETATM	2033	O	HOH	509	12.348	25.386	50.763	1.00	30.93	O
25	HETATM	2034	O	HOH	510	28.498	23.703	34.824	1.00	37.09	O
	HETATM	2035	O	HOH	511	26.394	10.521	64.086	1.00	30.68	O
	HETATM	2036	O	HOH	512	20.573	9.150	38.613	1.00	30.36	O
	HETATM	2037	O	HOH	513	19.724	30.629	29.203	1.00	35.40	O
	HETATM	2038	O	HOH	514	4.372	27.504	42.595	1.00	31.46	O
30	HETATM	2039	O	HOH	515	2.808	13.423	33.286	1.00	30.93	O
	HETATM	2040	O	HOH	516	23.698	20.154	43.135	1.00	37.92	O
	HETATM	2041	O	HOH	517	11.325	5.901	37.588	1.00	30.12	O
	HETATM	2042	O	HOH	518	0.885	13.049	59.537	1.00	39.32	O
	HETATM	2043	O	HOH	519	20.338	11.515	62.065	1.00	36.13	O
35	HETATM	2044	O	HOH	520	8.913	6.134	53.451	1.00	44.37	O
	HETATM	2045	O	HOH	521	4.924	23.321	44.129	1.00	33.51	O
	HETATM	2046	O	HOH	522	16.547	6.409	36.375	1.00	32.70	O
	HETATM	2047	O	HOH	523	8.896	35.918	45.789	1.00	45.73	O
	HETATM	2048	O	HOH	524	26.192	21.542	43.420	1.00	28.56	O
40	HETATM	2049	O	HOH	525	-5.345	32.214	23.915	1.00	35.31	O
	HETATM	2050	O	HOH	526	9.488	15.901	22.976	1.00	29.33	O
	HETATM	2051	O	HOH	527	5.345	31.465	22.796	1.00	31.37	O
	HETATM	2052	O	HOH	528	6.982	20.227	51.589	1.00	32.20	O
	HETATM	2053	O	HOH	529	4.642	13.886	30.953	1.00	31.71	O
45	HETATM	2054	O	HOH	530	-3.764	29.115	25.550	1.00	37.63	O
	HETATM	2055	O	HOH	531	31.831	9.097	66.550	1.00	36.20	O
	HETATM	2056	O	HOH	532	10.178	6.595	32.965	1.00	30.94	O
	HETATM	2057	O	HOH	533	-1.561	14.197	34.245	1.00	33.20	O
	HETATM	2058	O	HOH	534	0.476	12.154	62.160	1.00	39.93	O
50	HETATM	2059	O	HOH	535	25.970	5.142	53.011	1.00	47.31	O
	HETATM	2060	O	HOH	536	8.695	5.045	44.801	1.00	38.39	O
	HETATM	2061	O	HOH	537	22.396	11.047	39.112	1.00	40.45	O
	HETATM	2062	O	HOH	538	13.975	29.983	22.553	1.00	36.21	O
	HETATM	2063	O	HOH	539	-6.673	18.195	37.122	1.00	36.41	O
55	HETATM	2064	O	HOH	540	15.926	27.813	55.197	1.00	43.43	O
	HETATM	2065	O	HOH	541	21.922	29.786	26.625	1.00	39.42	O
	HETATM	2066	O	HOH	542	29.079	22.924	57.335	1.00	43.49	O
	HETATM	2067	O	HOH	543	-8.883	26.986	29.744	1.00	47.42	O
	HETATM	2068	O	HOH	544	-2.789	31.232	23.837	1.00	38.14	O

-166-

	HETATM 2069	O	HOH	545	15.578	33.329	45.128	1.00	39.44	O
	HETATM 2070	O	HOH	546	20.810	2.660	42.920	1.00	51.44	O
	HETATM 2071	O	HOH	547	27.448	25.982	58.310	1.00	43.04	O
5	HETATM 2072	O	HOH	548	21.987	8.152	64.287	1.00	43.15	O
	HETATM 2073	O	HOH	549	14.435	13.091	64.840	1.00	35.87	O
	HETATM 2074	O	HOH	550	1.276	25.772	21.944	1.00	40.66	O
	HETATM 2075	O	HOH	551	14.102	6.513	31.763	1.00	43.70	O
	HETATM 2076	O	HOH	552	11.990	24.017	53.147	1.00	45.62	O
10	HETATM 2077	O	HOH	553	3.481	24.236	20.666	1.00	35.69	O
	HETATM 2078	O	HOH	554	24.054	13.110	35.770	1.00	37.92	O
	HETATM 2079	O	HOH	556	6.857	37.182	44.351	1.00	49.60	O
	HETATM 2080	O	HOH	557	-8.644	30.901	30.925	1.00	41.21	O
	HETATM 2081	O	HOH	558	17.767	33.571	43.159	1.00	37.66	O
15	HETATM 2082	O	HOH	559	16.954	26.537	23.238	1.00	51.77	O
	HETATM 2083	O	HOH	560	27.386	20.638	40.959	1.00	37.25	O
	HETATM 2084	O	HOH	561	31.418	10.182	50.496	1.00	47.27	O
	HETATM 2085	O	HOH	562	4.082	21.082	20.610	1.00	37.94	O
	HETATM 2086	O	HOH	563	14.064	10.706	58.224	1.00	42.75	O
20	HETATM 2087	O	HOH	564	23.415	29.835	49.803	1.00	45.77	O
	HETATM 2088	O	HOH	565	14.533	11.393	24.395	1.00	36.60	O
	HETATM 2089	O	HOH	566	-0.868	36.798	40.025	1.00	52.17	O
	HETATM 2090	O	HOH	567	2.865	34.386	33.570	1.00	42.56	O
	HETATM 2091	O	HOH	568	-4.893	19.288	30.751	1.00	44.30	O
25	HETATM 2092	O	HOH	569	30.643	14.674	61.949	1.00	43.28	O
	HETATM 2093	O	HOH	570	22.702	3.372	47.417	1.00	36.93	O
	HETATM 2094	O	HOH	571	13.379	35.172	44.109	1.00	47.38	O
	HETATM 2095	O	HOH	572	-1.138	20.698	22.966	1.00	53.61	O
	HETATM 2096	O	HOH	573	25.589	19.849	33.401	1.00	52.13	O
30	HETATM 2097	O	HOH	574	23.893	13.360	32.579	1.00	45.26	O
	HETATM 2098	O	HOH	575	-7.367	18.485	31.944	1.00	48.23	O
	HETATM 2099	O	HOH	576	2.430	19.200	65.790	1.00	45.13	O
	HETATM 2100	O	HOH	577	20.048	32.028	44.907	1.00	46.82	O
	HETATM 2101	O	HOH	578	20.286	6.713	37.519	1.00	43.08	O
35	HETATM 2102	O	HOH	579	25.879	5.448	50.403	1.00	48.82	O
	HETATM 2103	O	HOH	580	24.905	19.763	39.659	1.00	45.39	O
	HETATM 2104	O	HOH	581	2.341	14.233	26.082	1.00	50.76	O
	HETATM 2105	O	HOH	582	15.248	20.000	60.506	1.00	44.08	O
	HETATM 2106	O	HOH	583	22.695	7.038	37.715	1.00	46.55	O
40	HETATM 2107	O	HOH	584	11.915	16.625	66.479	1.00	52.58	O
	HETATM 2108	O	HOH	585	20.145	35.730	35.936	1.00	46.90	O
	HETATM 2109	O	HOH	586	10.735	24.933	16.684	1.00	46.64	O
	HETATM 2110	O	HOH	587	1.182	9.495	61.830	1.00	55.88	O
	HETATM 2111	O	HOH	588	-3.993	16.527	51.745	1.00	43.33	O
45	HETATM 2112	O	HOH	589	21.842	29.919	56.624	1.00	42.17	O
	HETATM 2113	O	HOH	590	3.602	25.520	44.494	1.00	50.24	O
	HETATM 2114	O	HOH	591	1.198	23.984	44.777	1.00	43.76	O
	HETATM 2115	O	HOH	592	13.208	27.713	54.123	1.00	59.17	O
	HETATM 2116	O	HOH	593	27.958	7.530	50.434	1.00	53.55	O
	HETATM 2117	O	HOH	594	22.594	3.510	64.140	1.00	45.66	O
50	HETATM 2118	O	HOH	595	30.412	22.979	36.623	1.00	71.37	O
	HETATM 2119	O	HOH	596	10.560	15.906	20.574	1.00	50.32	O
	HETATM 2120	O	HOH	597	26.021	3.241	64.667	1.00	49.85	O
	HETATM 2121	O	HOH	598	19.853	9.062	62.967	1.00	56.45	O
	HETATM 2122	O	HOH	599	12.462	3.992	52.363	1.00	42.46	O
55	HETATM 2123	O	HOH	600	6.152	35.657	28.721	1.00	46.87	O
	HETATM 2124	O	HOH	601	7.626	29.983	53.085	1.00	51.73	O
	HETATM 2125	O	HOH	602	11.547	23.591	57.064	1.00	51.07	O
	HETATM 2126	O	HOH	603	24.407	19.393	31.035	1.00	53.85	O

-167-

	HETATM	2127	O	HOH	604	12.538	23.006	18.706	1.00	50.11	O
	HETATM	2128	O	HOH	605	1.839	16.469	66.997	1.00	49.40	O
	HETATM	2129	O	HOH	606	1.378	19.964	21.070	1.00	48.97	O
5	HETATM	2130	O	HOH	607	5.895	26.935	51.419	1.00	53.95	O
	HETATM	2131	O	HOH	608	13.122	33.698	19.464	1.00	52.90	O
	HETATM	2132	O	HOH	609	27.040	8.636	44.102	1.00	44.22	O
	HETATM	2133	O	HOH	610	18.833	30.775	55.879	1.00	54.75	O
	HETATM	2134	O	HOH	611	34.509	17.720	47.771	1.00	42.84	O
	HETATM	2135	O	HOH	612	18.356	32.644	25.579	1.00	42.52	O
10	HETATM	2136	O	HOH	613	-2.259	16.235	28.804	1.00	56.71	O
	HETATM	2137	O	HOH	614	16.400	38.404	21.700	1.00	46.19	O
	HETATM	2138	O	HOH	615	9.340	39.540	19.060	1.00	51.44	O
	HETATM	2139	O	HOH	616	20.026	35.074	32.855	1.00	47.06	O
	HETATM	2140	O	HOH	617	31.604	8.486	59.428	1.00	47.99	O
15	HETATM	2141	O	HOH	618	26.228	8.975	40.708	1.00	47.20	O
	HETATM	2142	O	HOH	619	0.460	15.378	28.064	1.00	50.21	O
	HETATM	2143	O	HOH	620	15.771	3.385	48.139	1.00	38.09	O
	HETATM	2144	O	HOH	621	25.135	17.914	42.644	1.00	60.05	O
	HETATM	2145	O	HOH	622	-2.286	29.197	21.618	1.00	53.99	O
20	HETATM	2146	O	HOH	623	32.865	18.926	45.658	1.00	48.11	O
	HETATM	2147	O	HOH	624	17.116	13.333	25.240	1.00	52.60	O
	HETATM	2148	O	HOH	625	-2.809	17.978	56.255	1.00	53.36	O
	HETATM	2149	O	HOH	626	-3.647	7.885	56.347	1.00	63.91	O
	HETATM	2150	O	HOH	627	17.746	24.596	21.608	1.00	59.81	O
25	HETATM	2151	O	HOH	628	28.368	5.841	47.861	1.00	66.08	O
	HETATM	2152	O	HOH	629	13.641	11.618	66.858	1.00	52.02	O
	HETATM	2153	O	HOH	630	8.052	20.893	16.742	1.00	53.91	O
	HETATM	2154	O	HOH	631	8.914	38.015	27.578	1.00	56.47	O
	HETATM	2155	O	HOH	632	9.081	13.482	19.627	1.00	57.14	O
30	HETATM	2156	O	HOH	633	-4.343	24.969	37.694	1.00	51.08	O
	HETATM	2157	O	HOH	634	3.597	28.859	46.576	1.00	54.80	O
	HETATM	2158	O	HOH	635	27.905	21.432	28.373	1.00	59.49	O
	HETATM	2159	O	HOH	636	-4.252	18.337	25.491	1.00	47.50	O
	HETATM	2160	O	HOH	637	-2.808	23.046	51.839	1.00	49.04	O
35	HETATM	2161	O	HOH	638	2.757	25.756	18.437	1.00	49.80	O
	HETATM	2162	O	HOH	639	15.470	7.390	63.803	1.00	52.42	O
	HETATM	2163	O	HOH	640	33.689	11.757	50.784	1.00	54.00	O
	HETATM	2164	O	HOH	641	6.223	13.352	20.927	1.00	49.77	O
	HETATM	2165	O	HOH	642	12.267	32.764	51.605	1.00	48.76	O
40	HETATM	2166	O	HOH	644	25.211	3.585	48.391	1.00	49.75	O
	HETATM	2167	O	HOH	645	0.619	24.002	51.358	1.00	49.46	O
	HETATM	2168	O	HOH	646	12.270	22.627	60.617	1.00	63.88	O
	HETATM	2169	O	HOH	647	0.202	23.805	47.834	1.00	52.54	O
	HETATM	2170	O	HOH	648	15.471	8.169	23.816	1.00	54.49	O
45	HETATM	2171	O	HOH	649	4.098	13.117	28.105	1.00	43.97	O
	HETATM	2172	O	HOH	650	16.032	4.857	59.064	1.00	55.67	O
	HETATM	2173	O	HOH	651	-5.591	11.911	55.960	1.00	63.35	O
	HETATM	2174	O	HOH	652	14.373	4.083	36.218	1.00	49.18	O
	HETATM	2175	O	HOH	653	11.138	5.501	59.825	1.00	51.19	O
50	HETATM	2176	O	HOH	654	26.262	1.299	50.288	1.00	61.20	O
	HETATM	2177	O	HOH	655	4.067	20.751	67.111	1.00	51.75	O
	HETATM	2178	O	HOH	656	11.291	34.551	23.646	1.00	53.35	O
	HETATM	2179	O	HOH	657	2.505	33.743	45.342	1.00	58.29	O
	HETATM	2180	O	HOH	658	18.881	-0.886	43.452	1.00	60.82	O
55	HETATM	2181	O	HOH	659	-1.930	13.191	62.255	1.00	65.05	O
	HETATM	2182	O	HOH	660	-3.587	12.153	34.625	1.00	51.24	O
	HETATM	2183	O	HOH	661	-2.064	26.008	58.110	1.00	58.94	O
	HETATM	2184	O	HOH	662	18.842	12.351	64.527	1.00	60.06	O

-168-

HETATM	2185	O	HOH	663	30.991	26.420	51.105	1.00	54.69	O
HETATM	2186	O	HOH	664	16.115	30.354	56.207	1.00	60.96	O
HETATM	2187	O	HOH	665	36.596	19.242	55.988	1.00	55.83	O

-169-

Table 3Atomic Structure Coordinate Data of
Polyalanine Model of Conserved VDR LBD

5	ATOM	1	CB	PRO	103	-17.052	-26.771	140.477	1.00	78.63	A	C
	ATOM	2	CG	PRO	103	-16.933	-28.077	141.262	1.00	78.57	A	C
	ATOM	3	C	PRO	103	-15.322	-25.595	139.088	1.00	78.42	A	C
10	ATOM	4	O	PRO	103	-15.845	-24.542	139.459	1.00	78.37	A	O
	ATOM	5	N	PRO	103	-14.952	-27.870	140.019	1.00	78.63	A	N
	ATOM	6	CD	PRO	103	-15.422	-28.350	141.331	1.00	78.61	A	C
	ATOM	7	CA	PRO	103	-15.952	-26.943	139.436	1.00	78.57	A	C
	ATOM	8	N	VAL	104	-14.202	-25.636	138.370	1.00	78.14	A	N
	ATOM	9	CA	VAL	104	-13.489	-24.422	137.982	1.00	77.74	A	C
15	ATOM	10	CB	VAL	104	-12.020	-24.729	137.584	1.00	77.77	A	C
	ATOM	11	CG1	VAL	104	-11.298	-25.415	138.733	1.00	77.66	A	C
	ATOM	12	CG2	VAL	104	-11.984	-25.591	136.331	1.00	77.68	A	C
	ATOM	13	C	VAL	104	-14.153	-23.671	136.828	1.00	77.43	A	C
	ATOM	14	O	VAL	104	-15.023	-24.202	136.133	1.00	77.67	A	O
20	ATOM	15	N	GLN	105	-13.726	-22.427	136.636	1.00	76.69	A	N
	ATOM	16	CA	GLN	105	-14.254	-21.567	135.582	1.00	75.70	A	C
	ATOM	17	CB	GLN	105	-13.976	-20.099	135.918	1.00	76.09	A	C
	ATOM	18	CG	GLN	105	-12.491	-19.779	136.067	1.00	76.08	A	C
	ATOM	19	CD	GLN	105	-12.210	-18.291	136.099	1.00	76.03	A	C
25	ATOM	20	OE1	GLN	105	-12.414	-17.589	135.107	1.00	75.85	A	O
	ATOM	21	NE2	GLN	105	-11.739	-17.800	137.241	1.00	75.74	A	N
	ATOM	22	C	GLN	105	-13.637	-21.877	134.223	1.00	74.59	A	C
	ATOM	23	O	GLN	105	-12.719	-22.691	134.111	1.00	74.90	A	O
	ATOM	24	N	LEU	106	-14.150	-21.211	133.193	1.00	72.98	A	N
30	ATOM	25	CA	LEU	106	-13.654	-21.381	131.836	1.00	71.07	A	C
	ATOM	26	CB	LEU	106	-14.603	-22.279	131.032	1.00	71.27	A	C
	ATOM	27	CG	LEU	106	-14.142	-22.724	129.638	1.00	71.35	A	C
	ATOM	28	CD1	LEU	106	-12.802	-23.437	129.733	1.00	71.22	A	C
	ATOM	29	CD2	LEU	106	-15.188	-23.645	129.027	1.00	71.16	A	C
35	ATOM	30	C	LEU	106	-13.537	-20.002	131.185	1.00	69.48	A	C
	ATOM	31	O	LEU	106	-14.517	-19.447	130.693	1.00	69.41	A	O
	ATOM	32	N	SER	107	-12.326	-19.456	131.211	1.00	67.67	A	N
	ATOM	33	CA	SER	107	-12.021	-18.145	130.645	1.00	65.85	A	C
	ATOM	34	CB	SER	107	-10.516	-18.043	130.383	1.00	65.62	A	C
40	ATOM	35	OG	SER	107	-10.198	-16.891	129.625	1.00	65.53	A	O
	ATOM	36	C	SER	107	-12.776	-17.828	129.360	1.00	64.86	A	C
	ATOM	37	O	SER	107	-13.087	-18.721	128.573	1.00	64.79	A	O
	ATOM	38	N	LYS	108	-13.074	-16.549	129.154	1.00	63.49	A	N
	ATOM	39	CA	LYS	108	-13.772	-16.121	127.948	1.00	62.43	A	C
45	ATOM	40	CB	LYS	108	-14.196	-14.650	128.055	1.00	62.56	A	C
	ATOM	41	CG	LYS	108	-15.668	-14.437	128.417	1.00	62.85	A	C
	ATOM	42	CD	LYS	108	-16.022	-15.032	129.776	1.00	63.11	A	C
	ATOM	43	CE	LYS	108	-17.482	-14.777	130.129	1.00	63.62	A	C
	ATOM	44	NZ	LYS	108	-17.861	-15.362	131.449	1.00	63.58	A	N
50	ATOM	45	C	LYS	108	-12.848	-16.305	126.750	1.00	61.42	A	C
	ATOM	46	O	LYS	108	-13.289	-16.672	125.661	1.00	61.44	A	O
	ATOM	47	N	GLU	109	-11.563	-16.047	126.959	1.00	60.15	A	N
	ATOM	48	CA	GLU	109	-10.580	-16.204	125.900	1.00	58.91	A	C
	ATOM	49	CB	GLU	109	-9.232	-15.655	126.358	1.00	59.90	A	C
55	ATOM	50	CG	GLU	109	-8.171	-15.661	125.279	1.00	61.96	A	C

-170-

	ATOM	51	CD	GLU	109	-6.868	-15.046	125.745	1.00	63.27	A	C
	ATOM	52	OE1	GLU	109	-6.885	-13.866	126.160	1.00	64.16	A	O
	ATOM	53	OE2	GLU	109	-5.829	-15.741	125.696	1.00	63.84	A	O
5	ATOM	54	C	GLU	109	-10.443	-17.682	125.524	1.00	57.30	A	C
	ATOM	55	O	GLU	109	-10.154	-18.014	124.376	1.00	56.66	A	O
	ATOM	56	N	GLN	110	-10.655	-18.560	126.499	1.00	55.60	A	N
	ATOM	57	CA	GLN	110	-10.564	-19.997	126.284	1.00	54.48	A	C
	ATOM	58	CB	GLN	110	-10.456	-20.723	127.626	1.00	53.38	A	C
10	ATOM	59	CG	GLN	110	-9.118	-20.512	128.310	1.00	52.62	A	C
	ATOM	60	CD	GLN	110	-9.004	-21.225	129.642	1.00	52.04	A	C
	ATOM	61	OE1	GLN	110	-7.901	-21.441	130.141	1.00	51.99	A	O
	ATOM	62	NE2	GLN	110	-10.141	-21.583	130.230	1.00	51.70	A	N
	ATOM	63	C	GLN	110	-11.754	-20.537	125.503	1.00	54.10	A	C
15	ATOM	64	O	GLN	110	-11.603	-21.426	124.671	1.00	53.77	A	O
	ATOM	65	N	GLU	111	-12.938	-20.001	125.772	1.00	53.80	A	N
	ATOM	66	CA	GLU	111	-14.130	-20.450	125.068	1.00	53.73	A	C
	ATOM	67	CB	GLU	111	-15.389	-19.943	125.774	1.00	54.85	A	C
	ATOM	68	CG	GLU	111	-15.607	-20.597	127.131	1.00	56.90	A	C
20	ATOM	69	CD	GLU	111	-16.899	-20.172	127.793	1.00	58.68	A	C
	ATOM	70	OE1	GLU	111	-17.970	-20.349	127.171	1.00	60.00	A	O
	ATOM	71	OE2	GLU	111	-16.846	-19.666	128.936	1.00	59.57	A	O
	ATOM	72	C	GLU	111	-14.112	-20.007	123.610	1.00	52.44	A	C
	ATOM	73	O	GLU	111	-14.672	-20.680	122.747	1.00	52.44	A	O
25	ATOM	74	N	GLU	112	-13.464	-18.880	123.334	1.00	50.93	A	N
	ATOM	75	CA	GLU	112	-13.367	-18.387	121.968	1.00	49.46	A	C
	ATOM	76	CB	GLU	112	-12.980	-16.909	121.956	1.00	50.56	A	C
	ATOM	77	CG	GLU	112	-14.044	-16.030	121.322	1.00	52.74	A	C
	ATOM	78	CD	GLU	112	-15.427	-16.308	121.887	1.00	53.94	A	C
30	ATOM	79	OE1	GLU	112	-15.634	-16.105	123.106	1.00	54.84	A	O
	ATOM	80	OE2	GLU	112	-16.306	-16.737	121.110	1.00	54.87	A	O
	ATOM	81	C	GLU	112	-12.332	-19.204	121.212	1.00	47.53	A	C
	ATOM	82	O	GLU	112	-12.470	-19.442	120.015	1.00	47.52	A	O
	ATOM	83	N	LEU	113	-11.290	-19.622	121.922	1.00	45.16	A	N
35	ATOM	84	CA	LEU	113	-10.236	-20.440	121.341	1.00	42.62	A	C
	ATOM	85	CB	LEU	113	-9.217	-20.822	122.418	1.00	42.09	A	C
	ATOM	86	CG	LEU	113	-7.813	-21.290	122.021	1.00	42.04	A	C
	ATOM	87	CD1	LEU	113	-7.183	-21.991	123.223	1.00	41.08	A	C
	ATOM	88	CD2	LEU	113	-7.861	-22.234	120.836	1.00	41.07	A	C
40	ATOM	89	C	LEU	113	-10.916	-21.704	120.824	1.00	41.07	A	C
	ATOM	90	O	LEU	113	-10.746	-22.096	119.670	1.00	39.68	A	O
	ATOM	91	N	ILE	114	-11.691	-22.327	121.706	1.00	39.49	A	N
	ATOM	92	CA	ILE	114	-12.416	-23.548	121.395	1.00	39.05	A	C
	ATOM	93	CB	ILE	114	-13.126	-24.082	122.660	1.00	37.48	A	C
	ATOM	94	CG2	ILE	114	-13.999	-25.273	122.313	1.00	37.05	A	C
45	ATOM	95	CG1	ILE	114	-12.075	-24.469	123.709	1.00	36.78	A	C
	ATOM	96	CD1	ILE	114	-12.648	-24.927	125.034	1.00	35.81	A	C
	ATOM	97	C	ILE	114	-13.431	-23.352	120.267	1.00	39.39	A	C
	ATOM	98	O	ILE	114	-13.632	-24.240	119.440	1.00	39.39	A	O
50	ATOM	99	N	ARG	115	-14.069	-22.190	120.229	1.00	39.79	A	N
	ATOM	100	CA	ARG	115	-15.045	-21.913	119.185	1.00	40.43	A	C
	ATOM	101	CB	ARG	115	-15.769	-20.598	119.473	1.00	42.33	A	C
	ATOM	102	CG	ARG	115	-16.842	-20.248	118.451	1.00	45.85	A	C
	ATOM	103	CD	ARG	115	-16.819	-18.762	118.113	1.00	49.10	A	C
55	ATOM	104	NE	ARG	115	-15.561	-18.376	117.470	1.00	51.76	A	N
	ATOM	105	CZ	ARG	115	-15.271	-17.146	117.053	1.00	52.78	A	C
	ATOM	106	NH1	ARG	115	-16.148	-16.163	117.207	1.00	53.95	A	N
	ATOM	107	NH2	ARG	115	-14.100	-16.899	116.478	1.00	53.49	A	N
	ATOM	108	C	ARG	115	-14.327	-21.824	117.839	1.00	39.30	A	C

-171-

5	ATOM	109	O	ARG	115	-14.794	-22.357	116.833	1.00	39.26	A	O
	ATOM	110	N	THR	116	-13.190	-21.140	117.831	1.00	37.95	A	N
	ATOM	111	CA	THR	116	-12.389	-20.979	116.626	1.00	36.97	A	C
	ATOM	112	CB	THR	116	-11.177	-20.076	116.900	1.00	37.51	A	C
	ATOM	113	OG1	THR	116	-11.625	-18.847	117.483	1.00	39.12	A	O
10	ATOM	114	CG2	THR	116	-10.434	-19.778	115.614	1.00	37.41	A	C
	ATOM	115	C	THR	116	-11.887	-22.332	116.122	1.00	35.58	A	C
	ATOM	116	O	THR	116	-11.905	-22.599	114.921	1.00	35.61	A	O
	ATOM	117	N	LEU	117	-11.434	-23.176	117.046	1.00	33.47	A	N
	ATOM	118	CA	LEU	117	-10.932	-24.500	116.705	1.00	31.78	A	C
15	ATOM	119	CB	LEU	117	-10.286	-25.143	117.929	1.00	30.67	A	C
	ATOM	120	CG	LEU	117	-8.959	-24.582	118.426	1.00	30.04	A	C
	ATOM	121	CD1	LEU	117	-8.543	-25.311	119.688	1.00	29.00	A	C
	ATOM	122	CD2	LEU	117	-7.905	-24.735	117.345	1.00	30.20	A	C
	ATOM	123	C	LEU	117	-12.041	-25.413	116.187	1.00	31.49	A	C
20	ATOM	124	O	LEU	117	-11.864	-26.112	115.195	1.00	31.28	A	O
	ATOM	125	N	LEU	118	-13.179	-25.413	116.876	1.00	31.24	A	N
	ATOM	126	CA	LEU	118	-14.320	-26.233	116.487	1.00	30.90	A	C
	ATOM	127	CB	LEU	118	-15.444	-26.091	117.510	1.00	30.93	A	C
	ATOM	128	CG	LEU	118	-15.173	-26.707	118.882	1.00	31.21	A	C
25	ATOM	129	CD1	LEU	118	-16.333	-26.391	119.819	1.00	31.43	A	C
	ATOM	130	CD2	LEU	118	-14.987	-28.210	118.737	1.00	30.10	A	C
	ATOM	131	C	LEU	118	-14.841	-25.848	115.111	1.00	30.73	A	C
	ATOM	132	O	LEU	118	-15.126	-26.713	114.287	1.00	30.25	A	O
	ATOM	133	N	GLY	119	-14.963	-24.544	114.872	1.00	30.45	A	N
30	ATOM	134	CA	GLY	119	-15.444	-24.067	113.586	1.00	29.84	A	C
	ATOM	135	C	GLY	119	-14.551	-24.519	112.445	1.00	29.41	A	C
	ATOM	136	O	GLY	119	-15.036	-24.986	111.411	1.00	29.26	A	O
	ATOM	137	N	ALA	120	-13.242	-24.383	112.634	1.00	28.27	A	N
	ATOM	138	CA	ALA	120	-12.277	-24.791	111.623	1.00	27.50	A	C
35	ATOM	139	CB	ALA	120	-10.887	-24.294	112.006	1.00	28.11	A	C
	ATOM	140	C	ALA	120	-12.273	-26.317	111.455	1.00	26.73	A	C
	ATOM	141	O	ALA	120	-12.223	-26.826	110.336	1.00	26.07	A	O
	ATOM	142	N	HIS	121	-12.348	-27.038	112.569	1.00	26.34	A	N
	ATOM	143	CA	HIS	121	-12.356	-28.498	112.542	1.00	25.51	A	C
40	ATOM	144	CB	HIS	121	-12.250	-29.053	113.967	1.00	25.42	A	C
	ATOM	145	CG	HIS	121	-12.478	-30.531	114.058	1.00	25.78	A	C
	ATOM	146	CD2	HIS	121	-11.622	-31.573	113.949	1.00	25.53	A	C
	ATOM	147	ND1	HIS	121	-13.729	-31.082	114.240	1.00	26.55	A	N
	ATOM	148	CE1	HIS	121	-13.633	-32.398	114.239	1.00	27.01	A	C
45	ATOM	149	NE2	HIS	121	-12.364	-32.723	114.064	1.00	27.07	A	N
	ATOM	150	C	HIS	121	-13.595	-29.068	111.857	1.00	25.65	A	C
	ATOM	151	O	HIS	121	-13.491	-29.943	111.000	1.00	23.32	A	O
	ATOM	152	N	THR	122	-14.769	-28.572	112.233	1.00	26.18	A	N
	ATOM	153	CA	THR	122	-16.013	-29.054	111.644	1.00	27.73	A	C
50	ATOM	154	CB	THR	122	-17.241	-28.391	112.310	1.00	27.99	A	C
	ATOM	155	OG1	THR	122	-17.135	-26.970	112.194	1.00	32.40	A	O
	ATOM	156	CG2	THR	122	-17.319	-28.750	113.780	1.00	27.74	A	C
	ATOM	157	C	THR	122	-16.063	-28.799	110.137	1.00	27.54	A	C
	ATOM	158	O	THR	122	-16.490	-29.657	109.368	1.00	26.85	A	O
55	ATOM	159	N	ARG	123	-15.598	-27.627	109.715	1.00	28.07	A	N
	ATOM	160	CA	ARG	123	-15.612	-27.269	108.300	1.00	29.18	A	C
	ATOM	161	CB	ARG	123	-15.349	-25.762	108.141	1.00	29.82	A	C
	ATOM	162	CG	ARG	123	-15.610	-25.226	106.727	1.00	33.27	A	C
	ATOM	163	CD	ARG	123	-15.159	-23.765	106.536	1.00	34.42	A	C
	ATOM	164	NE	ARG	123	-16.031	-22.773	107.179	1.00	36.89	A	N
	ATOM	165	CZ	ARG	123	-17.220	-22.381	106.714	1.00	36.96	A	C
	ATOM	166	NH1	ARG	123	-17.715	-22.888	105.592	1.00	37.38	A	N

-172-

	ATOM	167	NH2	ARG	123	-17.913	-21.458	107.366	1.00	37.20	A	N
	ATOM	168	C	ARG	123	-14.628	-28.055	107.415	1.00	28.35	A	C
	ATOM	169	O	ARG	123	-14.967	-28.431	106.290	1.00	27.61	A	O
5	ATOM	170	N	HIS	124	-13.426	-28.324	107.923	1.00	27.75	A	N
	ATOM	171	CA	HIS	124	-12.409	-29.016	107.125	1.00	27.66	A	C
	ATOM	172	CB	HIS	124	-11.148	-28.147	107.062	1.00	28.26	A	C
	ATOM	173	CG	HIS	124	-11.395	-26.764	106.543	1.00	29.25	A	C
	ATOM	174	CD2	HIS	124	-11.945	-26.333	105.382	1.00	28.40	A	C
10	ATOM	175	ND1	HIS	124	-11.081	-25.631	107.263	1.00	29.27	A	N
	ATOM	176	CE1	HIS	124	-11.426	-24.562	106.567	1.00	28.76	A	C
	ATOM	177	NE2	HIS	124	-11.953	-24.960	105.423	1.00	29.33	A	N
	ATOM	178	C	HIS	124	-11.982	-30.448	107.478	1.00	26.91	A	C
	ATOM	179	O	HIS	124	-11.534	-31.189	106.599	1.00	26.66	A	O
15	ATOM	180	N	MET	125	-12.118	-30.855	108.735	1.00	26.01	A	N
	ATOM	181	CA	MET	125	-11.659	-32.193	109.108	1.00	26.25	A	C
	ATOM	182	CB	MET	125	-10.443	-32.063	110.025	1.00	26.44	A	C
	ATOM	183	CG	MET	125	-9.325	-31.218	109.424	1.00	27.40	A	C
	ATOM	184	SD	MET	125	-7.795	-31.333	110.350	1.00	31.87	A	S
20	ATOM	185	CE	MET	125	-8.358	-30.864	111.998	1.00	31.61	A	C
	ATOM	186	C	MET	125	-12.657	-33.158	109.731	1.00	25.47	A	C
	ATOM	187	O	MET	125	-12.621	-34.355	109.446	1.00	25.35	A	O
	ATOM	188	N	GLY	126	-13.536	-32.641	110.581	1.00	24.84	A	N
	ATOM	189	CA	GLY	126	-14.524	-33.471	111.247	1.00	24.24	A	C
25	ATOM	190	C	GLY	126	-15.123	-34.597	110.426	1.00	23.67	A	C
	ATOM	191	O	GLY	126	-15.172	-35.739	110.883	1.00	23.66	A	O
	ATOM	192	N	THR	127	-15.581	-34.297	109.215	1.00	22.39	A	N
	ATOM	193	CA	THR	127	-16.177	-35.339	108.390	1.00	22.17	A	C
	ATOM	194	CB	THR	127	-17.667	-35.039	108.101	1.00	21.86	A	C
30	ATOM	195	OG1	THR	127	-17.787	-33.751	107.497	1.00	21.82	A	O
	ATOM	196	CG2	THR	127	-18.483	-35.056	109.387	1.00	22.67	A	C
	ATOM	197	C	THR	127	-15.463	-35.571	107.067	1.00	21.87	A	C
	ATOM	198	O	THR	127	-16.065	-36.071	106.118	1.00	21.50	A	O
	ATOM	199	N	MET	128	-14.179	-35.232	106.996	1.00	21.50	A	N
35	ATOM	200	CA	MET	128	-13.446	-35.420	105.746	1.00	21.52	A	C
	ATOM	201	CB	MET	128	-12.031	-34.823	105.845	1.00	22.11	A	C
	ATOM	202	CG	MET	128	-11.061	-35.562	106.770	1.00	22.14	A	C
	ATOM	203	SD	MET	128	-9.438	-34.750	106.857	1.00	21.82	A	S
	ATOM	204	CE	MET	128	-8.599	-35.832	108.065	1.00	22.47	A	C
40	ATOM	205	C	MET	128	-13.361	-36.881	105.315	1.00	21.38	A	C
	ATOM	206	O	MET	128	-13.211	-37.170	104.131	1.00	21.52	A	O
	ATOM	207	N	PHE	129	-13.463	-37.806	106.265	1.00	21.94	A	N
	ATOM	208	CA	PHE	129	-13.399	-39.231	105.939	1.00	21.94	A	C
	ATOM	209	CB	PHE	129	-13.509	-40.080	107.219	1.00	21.34	A	C
45	ATOM	210	CG	PHE	129	-14.896	-40.130	107.811	1.00	21.67	A	C
	ATOM	211	CD1	PHE	129	-15.849	-41.026	107.322	1.00	21.16	A	C
	ATOM	212	CD2	PHE	129	-15.251	-39.284	108.855	1.00	20.50	A	C
	ATOM	213	CE1	PHE	129	-17.137	-41.077	107.869	1.00	21.61	A	C
	ATOM	214	CE2	PHE	129	-16.533	-39.327	109.406	1.00	21.65	A	C
50	ATOM	215	CZ	PHE	129	-17.477	-40.225	108.912	1.00	21.57	A	C
	ATOM	216	C	PHE	129	-14.484	-39.644	104.938	1.00	21.50	A	C
	ATOM	217	O	PHE	129	-14.315	-40.613	104.197	1.00	20.88	A	O
	ATOM	218	N	GLU	130	-15.589	-38.906	104.911	1.00	21.77	A	N
	ATOM	219	CA	GLU	130	-16.686	-39.207	103.996	1.00	23.20	A	C
	ATOM	220	CB	GLU	130	-17.886	-38.307	104.298	1.00	23.75	A	C
55	ATOM	221	CG	GLU	130	-18.476	-38.533	105.681	1.00	26.72	A	C
	ATOM	222	CD	GLU	130	-19.666	-37.630	105.968	1.00	27.23	A	C
	ATOM	223	OE1	GLU	130	-19.938	-36.721	105.154	1.00	27.13	A	O
	ATOM	224	OE2	GLU	130	-20.321	-37.830	107.014	1.00	28.12	A	O

-173-

	ATOM	225	C	GLU	130	-16.313	-39.072	102.519	1.00	22.81	A	C
	ATOM	226	O	GLU	130	-17.020	-39.581	101.648	1.00	22.98	A	O
	ATOM	227	N	GLN	131	-15.211	-38.396	102.225	1.00	22.34	A	N
5	ATOM	228	CA	GLN	131	-14.826	-38.251	100.834	1.00	23.67	A	C
	ATOM	229	CB	GLN	131	-14.212	-36.864	100.579	1.00	25.71	A	C
	ATOM	230	CG	GLN	131	-14.915	-35.665	101.279	1.00	31.91	A	C
	ATOM	231	CD	GLN	131	-16.421	-35.495	100.986	1.00	35.53	A	C
	ATOM	232	OE1	GLN	131	-17.020	-34.490	101.382	1.00	39.09	A	O
10	ATOM	233	NE2	GLN	131	-17.033	-36.465	100.314	1.00	37.15	A	N
	ATOM	234	C	GLN	131	-13.871	-39.344	100.350	1.00	22.82	A	C
	ATOM	235	O	GLN	131	-13.486	-39.350	99.186	1.00	22.74	A	O
	ATOM	236	N	PHE	132	-13.500	-40.274	101.229	1.00	21.59	A	N
	ATOM	237	CA	PHE	132	-12.585	-41.345	100.840	1.00	20.93	A	C
15	ATOM	238	CB	PHE	132	-12.287	-42.289	102.023	1.00	19.90	A	C
	ATOM	239	CG	PHE	132	-11.445	-41.667	103.133	1.00	19.86	A	C
	ATOM	240	CD1	PHE	132	-10.858	-40.409	102.982	1.00	19.07	A	C
	ATOM	241	CD2	PHE	132	-11.258	-42.347	104.337	1.00	18.20	A	C
	ATOM	242	CE1	PHE	132	-10.104	-39.834	104.010	1.00	18.72	A	C
20	ATOM	243	CE2	PHE	132	-10.507	-41.783	105.371	1.00	18.68	A	C
	ATOM	244	CZ	PHE	132	-9.928	-40.525	105.211	1.00	18.24	A	C
	ATOM	245	C	PHE	132	-13.119	-42.169	99.658	1.00	20.71	A	C
	ATOM	246	O	PHE	132	-12.330	-42.675	98.861	1.00	20.20	A	O
	ATOM	247	N	VAL	133	-14.442	-42.300	99.538	1.00	20.69	A	N
25	ATOM	248	CA	VAL	133	-15.034	-43.076	98.438	1.00	22.08	A	C
	ATOM	249	CB	VAL	133	-16.554	-43.305	98.625	1.00	22.06	A	C
	ATOM	250	CG1	VAL	133	-16.799	-44.205	99.820	1.00	22.30	A	C
	ATOM	251	CG2	VAL	133	-17.281	-41.975	98.794	1.00	20.84	A	C
	ATOM	252	C	VAL	133	-14.825	-42.461	97.056	1.00	23.30	A	C
30	ATOM	253	O	VAL	133	-15.065	-43.110	96.040	1.00	21.98	A	O
	ATOM	254	N	GLN	134	-14.370	-41.214	97.028	1.00	25.25	A	N
	ATOM	255	CA	GLN	134	-14.110	-40.505	95.786	1.00	28.42	A	C
	ATOM	256	CB	GLN	134	-14.265	-39.001	95.992	1.00	31.35	A	C
	ATOM	257	CG	GLN	134	-15.676	-38.496	96.138	1.00	35.93	A	C
35	ATOM	258	CD	GLN	134	-15.692	-37.018	96.459	1.00	38.86	A	C
	ATOM	259	OE1	GLN	134	-14.978	-36.224	95.835	1.00	40.75	A	O
	ATOM	260	NE2	GLN	134	-16.510	-36.634	97.427	1.00	40.53	A	N
	ATOM	261	C	GLN	134	-12.701	-40.739	95.264	1.00	28.55	A	C
	ATOM	262	O	GLN	134	-12.305	-40.113	94.281	1.00	28.59	A	O
40	ATOM	263	N	PHE	135	-11.933	-41.612	95.911	1.00	27.76	A	N
	ATOM	264	CA	PHE	135	-10.562	-41.834	95.464	1.00	27.25	A	C
	ATOM	265	CB	PHE	135	-9.593	-41.361	96.556	1.00	27.33	A	C
	ATOM	266	CG	PHE	135	-9.653	-39.872	96.806	1.00	27.16	A	C
	ATOM	267	CD1	PHE	135	-9.062	-38.978	95.916	1.00	27.07	A	C
45	ATOM	268	CD2	PHE	135	-10.346	-39.363	97.900	1.00	27.37	A	C
	ATOM	269	CE1	PHE	135	-9.163	-37.595	96.110	1.00	26.82	A	C
	ATOM	270	CE2	PHE	135	-10.455	-37.979	98.104	1.00	27.26	A	C
	ATOM	271	CZ	PHE	135	-9.861	-37.096	97.206	1.00	26.50	A	C
	ATOM	272	C	PHE	135	-10.241	-43.256	95.022	1.00	26.66	A	C
50	ATOM	273	O	PHE	135	-9.247	-43.843	95.444	1.00	26.40	A	O
	ATOM	274	N	ARG	136	-11.086	-43.784	94.143	1.00	26.15	A	N
	ATOM	275	CA	ARG	136	-10.934	-45.129	93.586	1.00	25.96	A	C
	ATOM	276	CB	ARG	136	-9.900	-45.115	92.452	1.00	26.56	A	C
	ATOM	277	CG	ARG	136	-10.158	-44.063	91.372	1.00	29.01	A	C
55	ATOM	278	CD	ARG	136	-8.988	-43.086	91.285	1.00	31.35	A	C
	ATOM	279	NE	ARG	136	-9.452	-41.743	90.949	1.00	34.32	A	N
	ATOM	280	CZ	ARG	136	-8.939	-40.621	91.442	1.00	35.38	A	C
	ATOM	281	NH1	ARG	136	-7.934	-40.660	92.305	1.00	34.41	A	N
	ATOM	282	NH2	ARG	136	-9.442	-39.452	91.073	1.00	37.45	A	N

-174-

	ATOM	283	C	ARG	136	-10.530	-46.179	94.623	1.00	25.24	A	C
	ATOM	284	O	ARG	136	-9.486	-46.819	94.496	1.00	24.38	A	O
	ATOM	285	N	PRO	137	-11.357	-46.371	95.662	1.00	24.16	A	N
5	ATOM	286	CD	PRO	137	-12.632	-45.707	95.999	1.00	23.61	A	C
	ATOM	287	CA	PRO	137	-11.008	-47.366	96.672	1.00	23.41	A	C
	ATOM	288	CB	PRO	137	-11.999	-47.081	97.790	1.00	23.30	A	C
	ATOM	289	CG	PRO	137	-13.229	-46.654	97.013	1.00	23.80	A	C
	ATOM	290	C	PRO	137	-11.164	-48.776	96.149	1.00	23.31	A	C
10	ATOM	291	O	PRO	137	-12.181	-49.115	95.545	1.00	22.63	A	O
	ATOM	292	N	PRO	138	-10.147	-49.620	96.358	1.00	23.12	A	N
	ATOM	293	CD	PRO	138	-8.801	-49.369	96.907	1.00	23.19	A	C
	ATOM	294	CA	PRO	138	-10.283	-50.993	95.875	1.00	23.26	A	C
	ATOM	295	CB	PRO	138	-9.045	-51.679	96.450	1.00	23.98	A	C
15	ATOM	296	CG	PRO	138	-8.015	-50.578	96.421	1.00	24.11	A	C
	ATOM	297	C	PRO	138	-11.585	-51.547	96.464	1.00	22.75	A	C
	ATOM	298	O	PRO	138	-12.000	-51.142	97.556	1.00	22.46	A	O
	ATOM	299	N	ALA	139	-12.221	-52.468	95.748	1.00	21.31	A	N
	ATOM	300	CA	ALA	139	-13.475	-53.061	96.193	1.00	21.53	A	C
20	ATOM	301	CB	ALA	139	-14.001	-54.024	95.114	1.00	21.98	A	C
	ATOM	302	C	ALA	139	-13.442	-53.774	97.556	1.00	21.59	A	C
	ATOM	303	O	ALA	139	-14.439	-53.750	98.282	1.00	20.89	A	O
	ATOM	304	N	HIS	140	-12.320	-54.405	97.916	1.00	21.14	A	N
	ATOM	305	CA	HIS	140	-12.253	-55.107	99.199	1.00	21.89	A	C
25	ATOM	306	CB	HIS	140	-10.941	-55.903	99.342	1.00	22.63	A	C
	ATOM	307	CG	HIS	140	-9.759	-55.062	99.725	1.00	21.19	A	C
	ATOM	308	CD2	HIS	140	-9.227	-54.774	100.936	1.00	21.22	A	C
	ATOM	309	ND1	HIS	140	-9.024	-54.347	98.804	1.00	20.38	A	N
	ATOM	310	CE1	HIS	140	-8.094	-53.650	99.431	1.00	21.24	A	C
30	ATOM	311	NE2	HIS	140	-8.196	-53.890	100.726	1.00	22.01	A	N
	ATOM	312	C	HIS	140	-12.388	-54.153	100.392	1.00	22.47	A	C
	ATOM	313	O	HIS	140	-12.605	-54.586	101.518	1.00	22.16	A	O
	ATOM	314	N	LEU	141	-12.251	-52.857	100.134	1.00	23.58	A	N
	ATOM	315	CA	LEU	141	-12.364	-51.827	101.166	1.00	23.85	A	C
35	ATOM	316	CB	LEU	141	-11.777	-50.520	100.634	1.00	23.18	A	C
	ATOM	317	CG	LEU	141	-10.527	-49.937	101.294	1.00	24.27	A	C
	ATOM	318	CD1	LEU	141	-9.667	-51.037	101.903	1.00	22.26	A	C
	ATOM	319	CD2	LEU	141	-9.766	-49.121	100.262	1.00	21.25	A	C
	ATOM	320	C	LEU	141	-13.812	-51.599	101.603	1.00	24.27	A	C
40	ATOM	321	O	LEU	141	-14.066	-51.148	102.718	1.00	23.20	A	O
	ATOM	322	N	PHE	142	-14.759	-51.902	100.719	1.00	24.16	A	N
	ATOM	323	CA	PHE	142	-16.173	-51.717	101.032	1.00	25.36	A	C
	ATOM	324	CB	PHE	142	-17.017	-51.773	99.752	1.00	23.10	A	C
	ATOM	325	CG	PHE	142	-16.898	-50.549	98.901	1.00	22.13	A	C
45	ATOM	326	CD1	PHE	142	-17.570	-49.385	99.240	1.00	22.32	A	C
	ATOM	327	CD2	PHE	142	-16.087	-50.544	97.780	1.00	22.24	A	C
	ATOM	328	CE1	PHE	142	-17.432	-48.234	98.467	1.00	22.25	A	C
	ATOM	329	CE2	PHE	142	-15.944	-49.396	97.006	1.00	22.18	A	C
	ATOM	330	CZ	PHE	142	-16.615	-48.242	97.349	1.00	20.96	A	C
50	ATOM	331	C	PHE	142	-16.666	-52.771	102.005	1.00	26.65	A	C
	ATOM	332	O	PHE	142	-16.213	-53.914	101.976	1.00	26.20	A	O
	ATOM	333	N	ILE	143	-17.594	-52.380	102.873	1.00	28.79	A	N
	ATOM	334	CA	ILE	143	-18.165	-53.310	103.834	1.00	31.69	A	C
	ATOM	335	CB	ILE	143	-19.247	-52.630	104.743	1.00	32.78	A	C
55	ATOM	336	CG2	ILE	143	-18.682	-51.372	105.382	1.00	33.71	A	C
	ATOM	337	CG1	ILE	143	-20.516	-52.300	103.943	1.00	33.80	A	C
	ATOM	338	CD1	ILE	143	-20.373	-51.225	102.876	1.00	35.73	A	C
	ATOM	339	C	ILE	143	-18.814	-54.449	103.039	1.00	32.40	A	C
	ATOM	340	O	ILE	143	-19.161	-54.277	101.870	1.00	31.97	A	O

-175-

	ATOM	341	N	HIS	144	-18.967	-55.606	103.672	1.00	33.54	A	N
	ATOM	342	CA	HIS	144	-19.568	-56.769	103.023	1.00	35.74	A	C
	ATOM	343	CB	HIS	144	-20.924	-56.405	102.398	1.00	36.54	A	C
5	ATOM	344	CG	HIS	144	-21.853	-55.688	103.330	1.00	37.08	A	C
	ATOM	345	CD2	HIS	144	-22.508	-54.509	103.201	1.00	36.90	A	C
	ATOM	346	ND1	HIS	144	-22.207	-56.189	104.563	1.00	37.27	A	N
	ATOM	347	CE1	HIS	144	-23.037	-55.349	105.156	1.00	37.23	A	C
	ATOM	348	NE2	HIS	144	-23.235	-54.321	104.350	1.00	37.35	A	N
10	ATOM	349	C	HIS	144	-18.648	-57.317	101.932	1.00	36.21	A	C
	ATOM	350	O	HIS	144	-19.113	-57.751	100.877	1.00	36.04	A	O
	ATOM	351	N	HIS	145	-17.345	-57.289	102.191	1.00	37.47	A	N
	ATOM	352	CA	HIS	145	-16.356	-57.778	101.236	1.00	38.79	A	C
	ATOM	353	CB	HIS	145	-15.740	-56.611	100.471	1.00	38.32	A	C
15	ATOM	354	CG	HIS	145	-16.612	-56.082	99.379	1.00	38.92	A	C
	ATOM	355	CD2	HIS	145	-17.687	-55.260	99.416	1.00	38.33	A	C
	ATOM	356	ND1	HIS	145	-16.436	-56.427	98.056	1.00	38.61	A	N
	ATOM	357	CE1	HIS	145	-17.365	-55.840	97.325	1.00	38.59	A	C
	ATOM	358	NE2	HIS	145	-18.138	-55.127	98.125	1.00	39.24	A	N
20	ATOM	359	C	HIS	145	-15.248	-58.564	101.914	1.00	39.68	A	C
	ATOM	360	O	HIS	145	-14.995	-58.406	103.110	1.00	40.45	A	O
	ATOM	361	N	GLN	146	-14.593	-59.417	101.134	1.00	40.62	A	N
	ATOM	362	CA	GLN	146	-13.495	-60.232	101.632	1.00	40.83	A	C
	ATOM	363	CB	GLN	146	-13.470	-61.585	100.899	1.00	42.96	A	C
25	ATOM	364	CG	GLN	146	-13.528	-61.487	99.376	1.00	46.15	A	C
	ATOM	365	CD	GLN	146	-13.498	-62.850	98.685	1.00	48.68	A	C
	ATOM	366	OE1	GLN	146	-14.422	-63.659	98.824	1.00	49.88	A	O
	ATOM	367	NE2	GLN	146	-12.430	-63.105	97.934	1.00	49.37	A	N
	ATOM	368	C	GLN	146	-12.193	-59.464	101.412	1.00	39.30	A	C
30	ATOM	369	O	GLN	146	-12.075	-58.685	100.467	1.00	39.67	A	O
	ATOM	370	N	PRO	147	-11.201	-59.664	102.292	1.00	37.59	A	N
	ATOM	371	CD	PRO	147	-11.172	-60.620	103.411	1.00	37.45	A	C
	ATOM	372	CA	PRO	147	-9.917	-58.969	102.165	1.00	35.57	A	C
	ATOM	373	CB	PRO	147	-9.130	-59.485	103.367	1.00	36.50	A	C
35	ATOM	374	CG	PRO	147	-9.700	-60.851	103.580	1.00	37.77	A	C
	ATOM	375	C	PRO	147	-9.198	-59.208	100.835	1.00	33.38	A	C
	ATOM	376	O	PRO	147	-9.528	-60.134	100.094	1.00	33.33	A	O
	ATOM	377	N	LEU	148	-8.227	-58.353	100.535	1.00	30.98	A	N
	ATOM	378	CA	LEU	148	-7.448	-58.458	99.305	1.00	29.30	A	C
40	ATOM	379	CB	LEU	148	-6.282	-57.465	99.323	1.00	29.16	A	C
	ATOM	380	CG	LEU	148	-6.117	-56.372	98.263	1.00	29.82	A	C
	ATOM	381	CD1	LEU	148	-4.665	-55.910	98.289	1.00	29.71	A	C
	ATOM	382	CD2	LEU	148	-6.466	-56.870	96.883	1.00	29.27	A	C
	ATOM	383	C	LEU	148	-6.874	-59.865	99.153	1.00	27.66	A	C
45	ATOM	384	O	LEU	148	-6.281	-60.406	100.085	1.00	26.44	A	O
	ATOM	385	N	PRO	149	-7.057	-60.481	97.977	1.00	26.63	A	N
	ATOM	386	CD	PRO	149	-7.955	-60.093	96.877	1.00	26.30	A	C
	ATOM	387	CA	PRO	149	-6.523	-61.827	97.767	1.00	26.49	A	C
	ATOM	388	CB	PRO	149	-7.042	-62.192	96.376	1.00	26.48	A	C
50	ATOM	389	CG	PRO	149	-8.327	-61.433	96.288	1.00	26.76	A	C
	ATOM	390	C	PRO	149	-4.993	-61.798	97.824	1.00	26.14	A	C
	ATOM	391	O	PRO	149	-4.372	-60.749	97.645	1.00	26.17	A	O
	ATOM	392	N	THR	150	-4.402	-62.961	98.066	1.00	26.06	A	N
	ATOM	393	CA	THR	150	-2.955	-63.130	98.167	1.00	25.41	A	C
	ATOM	394	CB	THR	150	-2.605	-64.632	98.370	1.00	25.71	A	C
55	ATOM	395	OG1	THR	150	-2.981	-65.037	99.694	1.00	23.28	A	O
	ATOM	396	CG2	THR	150	-1.112	-64.888	98.148	1.00	25.10	A	C
	ATOM	397	C	THR	150	-2.173	-62.610	96.964	1.00	26.17	A	C
	ATOM	398	O	THR	150	-1.155	-61.933	97.123	1.00	25.67	A	O

-176-

	ATOM	399	N	LEU	151	-2.652	-62.924	95.766	1.00	26.09	A	N
	ATOM	400	CA	LEU	151	-1.973	-62.520	94.543	1.00	27.02	A	C
	ATOM	401	CB	LEU	151	-1.976	-63.692	93.548	1.00	28.10	A	C
5	ATOM	402	CG	LEU	151	-0.752	-64.622	93.469	1.00	28.68	A	C
	ATOM	403	CD1	LEU	151	-0.153	-64.874	94.830	1.00	28.89	A	C
	ATOM	404	CD2	LEU	151	-1.171	-65.927	92.809	1.00	28.50	A	C
	ATOM	405	C	LEU	151	-2.516	-61.258	93.865	1.00	26.77	A	C
	ATOM	406	O	LEU	151	-1.978	-60.827	92.849	1.00	26.56	A	O
10	ATOM	407	N	ALA	152	-3.565	-60.659	94.422	1.00	26.15	A	N
	ATOM	408	CA	ALA	152	-4.125	-59.442	93.836	1.00	25.48	A	C
	ATOM	409	CB	ALA	152	-5.423	-59.064	94.544	1.00	25.10	A	C
	ATOM	410	C	ALA	152	-3.121	-58.290	93.937	1.00	24.90	A	C
	ATOM	411	O	ALA	152	-2.517	-58.073	94.985	1.00	23.72	A	O
15	ATOM	412	N	PRO	153	-2.921	-57.544	92.841	1.00	24.54	A	N
	ATOM	413	CD	PRO	153	-3.389	-57.751	91.463	1.00	25.59	A	C
	ATOM	414	CA	PRO	153	-1.968	-56.435	92.919	1.00	24.98	A	C
	ATOM	415	CB	PRO	153	-1.970	-55.859	91.495	1.00	25.27	A	C
	ATOM	416	CG	PRO	153	-3.229	-56.374	90.870	1.00	25.95	A	C
20	ATOM	417	C	PRO	153	-2.368	-55.421	93.993	1.00	25.30	A	C
	ATOM	418	O	PRO	153	-3.554	-55.182	94.220	1.00	25.69	A	O
	ATOM	419	N	VAL	154	-1.376	-54.845	94.666	1.00	24.93	A	N
	ATOM	420	CA	VAL	154	-1.639	-53.884	95.730	1.00	25.63	A	C
	ATOM	421	CB	VAL	154	-0.608	-54.044	96.884	1.00	26.14	A	C
25	ATOM	422	CG1	VAL	154	0.737	-53.454	96.484	1.00	26.07	A	C
	ATOM	423	CG2	VAL	154	-1.129	-53.391	98.148	1.00	27.60	A	C
	ATOM	424	C	VAL	154	-1.644	-52.432	95.245	1.00	25.24	A	C
	ATOM	425	O	VAL	154	-2.049	-51.531	95.980	1.00	25.07	A	O
	ATOM	426	N	LEU	155	-1.200	-52.214	94.010	1.00	24.31	A	N
30	ATOM	427	CA	LEU	155	-1.150	-50.875	93.418	1.00	24.23	A	C
	ATOM	428	CB	LEU	155	-0.863	-50.977	91.910	1.00	24.21	A	C
	ATOM	429	CG	LEU	155	-0.776	-49.663	91.118	1.00	25.59	A	C
	ATOM	430	CD1	LEU	155	0.261	-48.739	91.744	1.00	24.34	A	C
	ATOM	431	CD2	LEU	155	-0.426	-49.962	89.658	1.00	24.80	A	C
35	ATOM	432	C	LEU	155	-2.418	-50.038	93.661	1.00	23.18	A	C
	ATOM	433	O	LEU	155	-2.335	-48.915	94.149	1.00	23.96	A	O
	ATOM	434	N	PRO	156	-3.607	-50.569	93.331	1.00	22.69	A	N
	ATOM	435	CD	PRO	156	-3.958	-51.848	92.684	1.00	22.19	A	C
	ATOM	436	CA	PRO	156	-4.808	-49.757	93.571	1.00	22.08	A	C
40	ATOM	437	CB	PRO	156	-5.944	-50.698	93.171	1.00	22.24	A	C
	ATOM	438	CG	PRO	156	-5.318	-51.539	92.086	1.00	22.14	A	C
	ATOM	439	C	PRO	156	-4.928	-49.277	95.031	1.00	22.20	A	C
	ATOM	440	O	PRO	156	-5.291	-48.122	95.287	1.00	20.87	A	O
	ATOM	441	N	LEU	157	-4.627	-50.164	95.980	1.00	20.93	A	N
45	ATOM	442	CA	LEU	157	-4.689	-49.813	97.397	1.00	20.80	A	C
	ATOM	443	CB	LEU	157	-4.433	-51.046	98.269	1.00	19.44	A	C
	ATOM	444	CG	LEU	157	-4.414	-50.793	99.783	1.00	19.55	A	C
	ATOM	445	CD1	LEU	157	-5.738	-50.152	100.220	1.00	16.57	A	C
	ATOM	446	CD2	LEU	157	-4.163	-52.113	100.522	1.00	16.20	A	C
50	ATOM	447	C	LEU	157	-3.657	-48.738	97.715	1.00	20.74	A	C
	ATOM	448	O	LEU	157	-3.950	-47.774	98.422	1.00	20.79	A	O
	ATOM	449	N	VAL	158	-2.450	-48.911	97.186	1.00	20.78	A	N
	ATOM	450	CA	VAL	158	-1.354	-47.962	97.387	1.00	20.77	A	C
	ATOM	451	CB	VAL	158	-0.061	-48.480	96.704	1.00	21.54	A	C
55	ATOM	452	CG1	VAL	158	1.014	-47.402	96.720	1.00	21.06	A	C
	ATOM	453	CG2	VAL	158	0.438	-49.743	97.420	1.00	20.78	A	C
	ATOM	454	C	VAL	158	-1.699	-46.583	96.810	1.00	21.47	A	C
	ATOM	455	O	VAL	158	-1.434	-45.549	97.428	1.00	21.74	A	O
	ATOM	456	N	THR	159	-2.293	-46.575	95.621	1.00	21.17	A	N

-177-

5	ATOM	457	CA	THR	159	-2.669	-45.334	94.956	1.00	21.04	A	C
	ATOM	458	CB	THR	159	-3.037	-45.606	93.484	1.00	21.88	A	C
	ATOM	459	OG1	THR	159	-2.012	-46.413	92.882	1.00	22.76	A	O
	ATOM	460	CG2	THR	159	-3.143	-44.308	92.710	1.00	21.05	A	C
	ATOM	461	C	THR	159	-3.841	-44.677	95.682	1.00	20.47	A	C
10	ATOM	462	O	THR	159	-3.944	-43.449	95.721	1.00	20.97	A	O
	ATOM	463	N	HIS	160	-4.721	-45.500	96.252	1.00	19.61	A	N
	ATOM	464	CA	HIS	160	-5.866	-45.009	97.008	1.00	20.01	A	C
	ATOM	465	CB	HIS	160	-6.789	-46.161	97.423	1.00	20.08	A	C
	ATOM	466	CG	HIS	160	-7.887	-45.744	98.354	1.00	20.94	A	C
15	ATOM	467	CD2	HIS	160	-8.085	-45.999	99.669	1.00	20.95	A	C
	ATOM	468	ND1	HIS	160	-8.925	-44.925	97.965	1.00	21.19	A	N
	ATOM	469	CE1	HIS	160	-9.713	-44.691	99.000	1.00	20.93	A	C
	ATOM	470	NE2	HIS	160	-9.225	-45.331	100.047	1.00	20.20	A	N
	ATOM	471	C	HIS	160	-5.328	-44.308	98.254	1.00	19.95	A	C
20	ATOM	472	O	HIS	160	-5.784	-43.219	98.600	1.00	20.42	A	O
	ATOM	473	N	PHE	161	-4.355	-44.933	98.920	1.00	18.59	A	N
	ATOM	474	CA	PHE	161	-3.736	-44.345	100.105	1.00	18.56	A	C
	ATOM	475	CB	PHE	161	-2.737	-45.327	100.735	1.00	18.23	A	C
	ATOM	476	CG	PHE	161	-3.368	-46.356	101.640	1.00	17.32	A	C
25	ATOM	477	CD1	PHE	161	-4.720	-46.314	101.941	1.00	16.89	A	C
	ATOM	478	CD2	PHE	161	-2.594	-47.362	102.206	1.00	18.24	A	C
	ATOM	479	CE1	PHE	161	-5.294	-47.255	102.792	1.00	17.84	A	C
	ATOM	480	CE2	PHE	161	-3.160	-48.308	103.058	1.00	17.78	A	C
	ATOM	481	CZ	PHE	161	-4.517	-48.253	103.352	1.00	16.70	A	C
30	ATOM	482	C	PHE	161	-3.018	-43.030	99.758	1.00	19.43	A	C
	ATOM	483	O	PHE	161	-3.122	-42.041	100.488	1.00	18.14	A	O
	ATOM	484	N	ALA	162	-2.281	-43.019	98.651	1.00	19.79	A	N
	ATOM	485	CA	ALA	162	-1.580	-41.809	98.233	1.00	21.41	A	C
	ATOM	486	CB	ALA	162	-0.818	-42.061	96.923	1.00	20.88	A	C
35	ATOM	487	C	ALA	162	-2.598	-40.674	98.040	1.00	22.02	A	C
	ATOM	488	O	ALA	162	-2.373	-39.545	98.471	1.00	22.29	A	O
	ATOM	489	N	ASP	163	-3.718	-40.991	97.399	1.00	22.30	A	N
	ATOM	490	CA	ASP	163	-4.766	-40.012	97.144	1.00	22.87	A	C
	ATOM	491	CB	ASP	163	-5.841	-40.626	96.236	1.00	23.81	A	C
40	ATOM	492	CG	ASP	163	-5.360	-40.804	94.788	1.00	25.70	A	C
	ATOM	493	OD1	ASP	163	-5.966	-41.605	94.044	1.00	24.91	A	O
	ATOM	494	OD2	ASP	163	-4.380	-40.134	94.390	1.00	25.54	A	O
	ATOM	495	C	ASP	163	-5.399	-39.468	98.426	1.00	23.27	A	C
	ATOM	496	O	ASP	163	-5.426	-38.254	98.633	1.00	22.56	A	O
45	ATOM	497	N	ILE	164	-5.896	-40.346	99.300	1.00	22.58	A	N
	ATOM	498	CA	ILE	164	-6.515	-39.858	100.527	1.00	22.00	A	C
	ATOM	499	CB	ILE	164	-7.329	-40.966	101.261	1.00	21.65	A	C
	ATOM	500	CG2	ILE	164	-8.363	-41.551	100.302	1.00	19.34	A	C
	ATOM	501	CG1	ILE	164	-6.409	-42.064	101.807	1.00	20.52	A	C
50	ATOM	502	CD1	ILE	164	-7.172	-43.169	102.530	1.00	18.21	A	C
	ATOM	503	C	ILE	164	-5.524	-39.207	101.490	1.00	22.19	A	C
	ATOM	504	O	ILE	164	-5.913	-38.346	102.281	1.00	21.74	A	O
	ATOM	505	N	ASN	165	-4.252	-39.599	101.425	1.00	21.86	A	N
	ATOM	506	CA	ASN	165	-3.241	-38.988	102.289	1.00	22.10	A	C
55	ATOM	507	CB	ASN	165	-1.899	-39.729	102.200	1.00	20.87	A	C
	ATOM	508	CG	ASN	165	-1.897	-41.047	102.962	1.00	21.09	A	C
	ATOM	509	OD1	ASN	165	-2.778	-41.308	103.784	1.00	19.71	A	O
	ATOM	510	ND2	ASN	165	-0.890	-41.880	102.703	1.00	19.72	A	N
	ATOM	511	C	ASN	165	-3.045	-37.534	101.858	1.00	22.73	A	C
	ATOM	512	O	ASN	165	-2.989	-36.628	102.690	1.00	22.46	A	O
	ATOM	513	N	THR	166	-2.932	-37.327	100.549	1.00	23.63	A	N
	ATOM	514	CA	THR	166	-2.758	-35.994	99.975	1.00	24.53	A	C

-178-

	ATOM	515	CB	THR	166	-2.564	-36.082	98.448	1.00	25.05	A	C
	ATOM	516	OG1	THR	166	-1.374	-36.830	98.166	1.00	25.95	A	O
	ATOM	517	CG2	THR	166	-2.451	-34.689	97.834	1.00	24.40	A	C
5	ATOM	518	C	THR	166	-4.002	-35.168	100.281	1.00	24.71	A	C
	ATOM	519	O	THR	166	-3.911	-34.020	100.727	1.00	25.33	A	O
	ATOM	520	N	PHE	167	-5.165	-35.765	100.034	1.00	23.87	A	N
	ATOM	521	CA	PHE	167	-6.438	-35.125	100.310	1.00	23.69	A	C
	ATOM	522	CB	PHE	167	-7.576	-36.132	100.111	1.00	23.28	A	C
10	ATOM	523	CG	PHE	167	-8.884	-35.699	100.719	1.00	23.25	A	C
	ATOM	524	CD1	PHE	167	-9.600	-34.629	100.184	1.00	23.28	A	C
	ATOM	525	CD2	PHE	167	-9.390	-36.351	101.842	1.00	22.82	A	C
	ATOM	526	CE1	PHE	167	-10.800	-34.213	100.757	1.00	21.97	A	C
	ATOM	527	CE2	PHE	167	-10.589	-35.946	102.427	1.00	22.68	A	C
15	ATOM	528	CZ	PHE	167	-11.298	-34.872	101.880	1.00	22.73	A	C
	ATOM	529	C	PHE	167	-6.440	-34.611	101.755	1.00	24.07	A	C
	ATOM	530	O	PHE	167	-6.676	-33.427	101.996	1.00	24.74	A	O
	ATOM	531	N	MET	168	-6.161	-35.508	102.702	1.00	22.88	A	N
	ATOM	532	CA	MET	168	-6.133	-35.168	104.123	1.00	22.54	A	C
20	ATOM	533	CB	MET	168	-5.844	-36.420	104.974	1.00	20.50	A	C
	ATOM	534	CG	MET	168	-7.020	-37.378	105.090	1.00	19.43	A	C
	ATOM	535	SD	MET	168	-6.792	-38.627	106.404	1.00	16.80	A	S
	ATOM	536	CE	MET	168	-5.899	-39.880	105.499	1.00	19.32	A	C
	ATOM	537	C	MET	168	-5.137	-34.065	104.472	1.00	22.25	A	C
25	ATOM	538	O	MET	168	-5.459	-33.160	105.226	1.00	21.58	A	O
	ATOM	539	N	VAL	169	-3.928	-34.144	103.932	1.00	22.92	A	N
	ATOM	540	CA	VAL	169	-2.927	-33.112	104.186	1.00	23.69	A	C
	ATOM	541	CB	VAL	169	-1.635	-33.375	103.383	1.00	24.08	A	C
	ATOM	542	CG1	VAL	169	-0.668	-32.208	103.555	1.00	25.04	A	C
30	ATOM	543	CG2	VAL	169	-0.981	-34.661	103.863	1.00	24.66	A	C
	ATOM	544	C	VAL	169	-3.470	-31.733	103.794	1.00	24.06	A	C
	ATOM	545	O	VAL	169	-3.335	-30.759	104.546	1.00	23.08	A	O
	ATOM	546	N	LEU	170	-4.084	-31.656	102.616	1.00	24.09	A	N
	ATOM	547	CA	LEU	170	-4.650	-30.404	102.131	1.00	24.47	A	C
35	ATOM	548	CB	LEU	170	-5.170	-30.587	100.702	1.00	25.76	A	C
	ATOM	549	CG	LEU	170	-4.109	-30.969	99.660	1.00	27.02	A	C
	ATOM	550	CD1	LEU	170	-4.776	-31.173	98.303	1.00	27.49	A	C
	ATOM	551	CD2	LEU	170	-3.037	-29.881	99.575	1.00	27.84	A	C
	ATOM	552	C	LEU	170	-5.772	-29.919	103.054	1.00	24.53	A	C
40	ATOM	553	O	LEU	170	-5.954	-28.715	103.246	1.00	24.40	A	O
	ATOM	554	N	GLN	171	-6.519	-30.855	103.637	1.00	23.66	A	N
	ATOM	555	CA	GLN	171	-7.589	-30.484	104.550	1.00	23.20	A	C
	ATOM	556	CB	GLN	171	-8.482	-31.692	104.856	1.00	22.89	A	C
	ATOM	557	CG	GLN	171	-9.301	-32.169	103.657	1.00	22.15	A	C
45	ATOM	558	CD	GLN	171	-10.227	-31.085	103.108	1.00	21.39	A	C
	ATOM	559	OE1	GLN	171	-11.164	-30.644	103.777	1.00	20.79	A	O
	ATOM	560	NE2	GLN	171	-9.960	-30.650	101.888	1.00	20.38	A	N
	ATOM	561	C	GLN	171	-7.004	-29.920	105.841	1.00	23.71	A	C
	ATOM	562	O	GLN	171	-7.621	-29.071	106.485	1.00	22.77	A	O
50	ATOM	563	N	VAL	172	-5.820	-30.390	106.232	1.00	24.17	A	N
	ATOM	564	CA	VAL	172	-5.195	-29.868	107.445	1.00	25.12	A	C
	ATOM	565	CB	VAL	172	-3.989	-30.714	107.893	1.00	25.29	A	C
	ATOM	566	CG1	VAL	172	-3.268	-30.005	109.034	1.00	23.34	A	C
	ATOM	567	CG2	VAL	172	-4.450	-32.098	108.339	1.00	24.47	A	C
	ATOM	568	C	VAL	172	-4.711	-28.440	107.193	1.00	25.52	A	C
55	ATOM	569	O	VAL	172	-4.833	-27.565	108.057	1.00	25.32	A	O
	ATOM	570	N	ILE	173	-4.149	-28.215	106.010	1.00	26.12	A	N
	ATOM	571	CA	ILE	173	-3.663	-26.895	105.646	1.00	26.88	A	C
	ATOM	572	CB	ILE	173	-3.062	-26.902	104.231	1.00	26.76	A	C

-179-

	ATOM	573	CG2	ILE	173	-2.686	-25.491	103.822	1.00	26.79	A	C
	ATOM	574	CG1	ILE	173	-1.835	-27.822	104.208	1.00	27.16	A	C
	ATOM	575	CD1	ILE	173	-1.135	-27.937	102.866	1.00	27.08	A	C
5	ATOM	576	C	ILE	173	-4.837	-25.919	105.718	1.00	27.47	A	C
	ATOM	577	O	ILE	173	-4.729	-24.847	106.320	1.00	27.14	A	O
	ATOM	578	N	LYS	174	-5.962	-26.305	105.122	1.00	27.73	A	N
	ATOM	579	CA	LYS	174	-7.162	-25.473	105.141	1.00	28.31	A	C
	ATOM	580	CB	LYS	174	-8.264	-26.123	104.296	1.00	28.44	A	C
10	ATOM	581	CG	LYS	174	-7.935	-26.108	102.803	1.00	29.80	A	C
	ATOM	582	CD	LYS	174	-8.878	-26.964	101.975	1.00	31.27	A	C
	ATOM	583	CE	LYS	174	-10.279	-26.412	101.958	1.00	32.16	A	C
	ATOM	584	NZ	LYS	174	-11.147	-27.278	101.116	1.00	34.46	A	N
	ATOM	585	C	LYS	174	-7.647	-25.232	106.570	1.00	28.11	A	C
15	ATOM	586	O	LYS	174	-8.142	-24.147	106.885	1.00	28.60	A	O
	ATOM	587	N	PHE	175	-7.499	-26.240	107.429	1.00	27.63	A	N
	ATOM	588	CA	PHE	175	-7.898	-26.142	108.834	1.00	27.68	A	C
	ATOM	589	CB	PHE	175	-7.736	-27.507	109.524	1.00	27.35	A	C
	ATOM	590	CG	PHE	175	-7.842	-27.452	111.029	1.00	27.54	A	C
20	ATOM	591	CD1	PHE	175	-9.041	-27.119	111.651	1.00	27.14	A	C
	ATOM	592	CD2	PHE	175	-6.730	-27.709	111.822	1.00	27.58	A	C
	ATOM	593	CE1	PHE	175	-9.129	-27.040	113.039	1.00	26.74	A	C
	ATOM	594	CE2	PHE	175	-6.806	-27.632	113.215	1.00	27.74	A	C
	ATOM	595	CZ	PHE	175	-8.010	-27.296	113.823	1.00	27.47	A	C
25	ATOM	596	C	PHE	175	-7.042	-25.094	109.551	1.00	28.52	A	C
	ATOM	597	O	PHE	175	-7.558	-24.244	110.268	1.00	27.62	A	O
	ATOM	598	N	THR	176	-5.731	-25.148	109.343	1.00	29.79	A	N
	ATOM	599	CA	THR	176	-4.824	-24.204	109.985	1.00	31.23	A	C
	ATOM	600	CB	THR	176	-3.358	-24.621	109.789	1.00	30.67	A	C
30	ATOM	601	OG1	THR	176	-3.022	-24.563	108.399	1.00	30.30	A	O
	ATOM	602	CG2	THR	176	-3.138	-26.036	110.306	1.00	31.22	A	C
	ATOM	603	C	THR	176	-4.998	-22.774	109.479	1.00	32.33	A	C
	ATOM	604	O	THR	176	-4.812	-21.819	110.232	1.00	32.61	A	O
	ATOM	605	N	LYS	177	-5.358	-22.633	108.207	1.00	33.30	A	N
35	ATOM	606	CA	LYS	177	-5.565	-21.319	107.602	1.00	34.34	A	C
	ATOM	607	CB	LYS	177	-5.823	-21.465	106.105	1.00	35.54	A	C
	ATOM	608	CG	LYS	177	-4.625	-21.950	105.310	1.00	38.15	A	C
	ATOM	609	CD	LYS	177	-3.612	-20.844	105.087	1.00	39.75	A	C
	ATOM	610	CE	LYS	177	-2.354	-21.393	104.434	1.00	40.78	A	C
40	ATOM	611	NZ	LYS	177	-2.655	-22.148	103.187	1.00	41.40	A	N
	ATOM	612	C	LYS	177	-6.732	-20.572	108.243	1.00	34.59	A	C
	ATOM	613	O	LYS	177	-6.806	-19.345	108.153	1.00	35.04	A	O
	ATOM	614	N	ASP	178	-7.642	-21.314	108.874	1.00	34.14	A	N
	ATOM	615	CA	ASP	178	-8.802	-20.730	109.543	1.00	34.02	A	C
45	ATOM	616	CB	ASP	178	-10.006	-21.668	109.445	1.00	34.24	A	C
	ATOM	617	CG	ASP	178	-10.744	-21.539	108.129	1.00	34.92	A	C
	ATOM	618	OD1	ASP	178	-10.332	-20.726	107.277	1.00	35.28	A	O
	ATOM	619	OD2	ASP	178	-11.749	-22.252	107.950	1.00	36.67	A	O
	ATOM	620	C	ASP	178	-8.542	-20.419	111.013	1.00	33.84	A	C
50	ATOM	621	O	ASP	178	-9.468	-20.085	111.752	1.00	34.10	A	O
	ATOM	622	N	LEU	179	-7.288	-20.542	111.439	1.00	33.64	A	N
	ATOM	623	CA	LEU	179	-6.916	-20.262	112.819	1.00	33.48	A	C
	ATOM	624	CB	LEU	179	-6.100	-21.420	113.398	1.00	32.20	A	C
	ATOM	625	CG	LEU	179	-6.695	-22.827	113.240	1.00	31.98	A	C
55	ATOM	626	CD1	LEU	179	-5.809	-23.831	113.963	1.00	31.56	A	C
	ATOM	627	CD2	LEU	179	-8.107	-22.876	113.793	1.00	30.73	A	C
	ATOM	628	C	LEU	179	-6.090	-18.981	112.834	1.00	33.94	A	C
	ATOM	629	O	LEU	179	-4.913	-18.982	112.464	1.00	33.94	A	O
	ATOM	630	N	PRO	180	-6.703	-17.863	113.252	1.00	34.34	A	N

-180-

	ATOM	631	CD	PRO	180	-8.097	-17.743	113.718	1.00	34.10	A	C
	ATOM	632	CA	PRO	180	-6.028	-16.564	113.312	1.00	34.65	A	C
	ATOM	633	CB	PRO	180	-6.994	-15.725	114.135	1.00	34.81	A	C
5	ATOM	634	CG	PRO	180	-8.322	-16.250	113.675	1.00	34.48	A	C
	ATOM	635	C	PRO	180	-4.631	-16.606	113.916	1.00	35.01	A	C
	ATOM	636	O	PRO	180	-3.680	-16.112	113.320	1.00	34.47	A	O
	ATOM	637	N	VAL	181	-4.501	-17.208	115.092	1.00	35.81	A	N
	ATOM	638	CA	VAL	181	-3.200	-17.275	115.745	1.00	36.75	A	C
10	ATOM	639	CB	VAL	181	-3.311	-17.889	117.149	1.00	37.21	A	C
	ATOM	640	CG1	VAL	181	-1.931	-18.014	117.762	1.00	38.68	A	C
	ATOM	641	CG2	VAL	181	-4.189	-17.007	118.032	1.00	38.14	A	C
	ATOM	642	C	VAL	181	-2.165	-18.051	114.935	1.00	36.94	A	C
	ATOM	643	O	VAL	181	-0.978	-17.730	114.976	1.00	36.68	A	O
15	ATOM	644	N	PHE	182	-2.604	-19.069	114.198	1.00	37.05	A	N
	ATOM	645	CA	PHE	182	-1.677	-19.847	113.378	1.00	37.75	A	C
	ATOM	646	CB	PHE	182	-2.325	-21.141	112.878	1.00	37.39	A	C
	ATOM	647	CG	PHE	182	-1.431	-21.945	111.972	1.00	37.39	A	C
	ATOM	648	CD1	PHE	182	-0.475	-22.806	112.500	1.00	37.05	A	C
20	ATOM	649	CD2	PHE	182	-1.513	-21.805	110.590	1.00	37.20	A	C
	ATOM	650	CE1	PHE	182	0.387	-23.517	111.663	1.00	36.56	A	C
	ATOM	651	CE2	PHE	182	-0.653	-22.511	109.746	1.00	37.00	A	C
	ATOM	652	CZ	PHE	182	0.297	-23.368	110.286	1.00	36.96	A	C
	ATOM	653	C	PHE	182	-1.242	-19.036	112.163	1.00	38.08	A	C
25	ATOM	654	O	PHE	182	-0.063	-18.976	111.826	1.00	37.90	A	O
	ATOM	655	N	ARG	183	-2.214	-18.426	111.499	1.00	39.10	A	N
	ATOM	656	CA	ARG	183	-1.948	-17.630	110.314	1.00	40.37	A	C
	ATOM	657	CB	ARG	183	-3.268	-17.242	109.661	1.00	40.60	A	C
	ATOM	658	CG	ARG	183	-3.094	-16.612	108.314	1.00	41.01	A	C
30	ATOM	659	CD	ARG	183	-4.196	-17.041	107.394	1.00	40.77	A	C
	ATOM	660	NE	ARG	183	-4.070	-16.387	106.101	1.00	40.69	A	N
	ATOM	661	CZ	ARG	183	-5.001	-16.419	105.160	1.00	39.62	A	C
	ATOM	662	NH1	ARG	183	-6.132	-17.079	105.370	1.00	39.80	A	N
	ATOM	663	NH2	ARG	183	-4.800	-15.783	104.017	1.00	38.99	A	N
35	ATOM	664	C	ARG	183	-1.129	-16.381	110.618	1.00	41.43	A	C
	ATOM	665	O	ARG	183	-0.433	-15.856	109.747	1.00	41.39	A	O
	ATOM	666	N	SER	184	-1.215	-15.910	111.858	1.00	42.46	A	N
	ATOM	667	CA	SER	184	-0.484	-14.728	112.292	1.00	43.82	A	C
	ATOM	668	CB	SER	184	-1.051	-14.236	113.620	1.00	44.39	A	C
40	ATOM	669	OG	SER	184	-0.499	-12.984	113.959	1.00	47.04	A	O
	ATOM	670	C	SER	184	1.016	-14.996	112.439	1.00	44.32	A	C
	ATOM	671	O	SER	184	1.813	-14.060	112.538	1.00	44.62	A	O
	ATOM	672	N	LEU	185	1.395	-16.273	112.459	1.00	44.27	A	N
	ATOM	673	CA	LEU	185	2.796	-16.666	112.578	1.00	44.64	A	C
45	ATOM	674	CB	LEU	185	2.903	-18.150	112.945	1.00	43.86	A	C
	ATOM	675	CG	LEU	185	2.344	-18.644	114.282	1.00	44.09	A	C
	ATOM	676	CD1	LEU	185	2.459	-20.166	114.362	1.00	42.72	A	C
	ATOM	677	CD2	LEU	185	3.103	-17.992	115.423	1.00	43.21	A	C
	ATOM	678	C	LEU	185	3.510	-16.447	111.248	1.00	45.42	A	C
50	ATOM	679	O	LEU	185	2.876	-16.405	110.194	1.00	45.54	A	O
	ATOM	680	N	PRO	186	4.844	-16.304	111.278	1.00	46.26	A	N
	ATOM	681	CD	PRO	186	5.775	-16.356	112.418	1.00	46.30	A	C
	ATOM	682	CA	PRO	186	5.566	-16.103	110.018	1.00	46.87	A	C
	ATOM	683	CB	PRO	186	7.008	-15.893	110.477	1.00	46.47	A	C
55	ATOM	684	CG	PRO	186	7.084	-16.693	111.741	1.00	47.00	A	C
	ATOM	685	C	PRO	186	5.390	-17.348	109.144	1.00	47.62	A	C
	ATOM	686	O	PRO	186	5.308	-18.463	109.659	1.00	48.13	A	O
	ATOM	687	N	ILE	187	5.328	-17.154	107.830	1.00	47.94	A	N
	ATOM	688	CA	ILE	187	5.131	-18.256	106.891	1.00	47.82	A	C

-181-

	ATOM	689	CB	ILE	187	5.236	-17.749	105.423	1.00	48.13	A	C
	ATOM	690	CG2	ILE	187	6.601	-17.105	105.182	1.00	48.93	A	C
	ATOM	691	CG1	ILE	187	4.975	-18.895	104.442	1.00	48.18	A	C
5	ATOM	692	CD1	ILE	187	6.169	-19.808	104.180	1.00	48.34	A	C
	ATOM	693	C	ILE	187	6.055	-19.460	107.095	1.00	47.81	A	C
	ATOM	694	O	ILE	187	5.614	-20.602	106.967	1.00	47.87	A	O
	ATOM	695	N	GLU	188	7.327	-19.221	107.405	1.00	47.20	A	N
	ATOM	696	CA	GLU	188	8.265	-20.320	107.619	1.00	46.46	A	C
10	ATOM	697	CB	GLU	188	9.702	-19.800	107.799	1.00	47.64	A	C
	ATOM	698	CG	GLU	188	9.846	-18.469	108.533	1.00	50.01	A	C
	ATOM	699	CD	GLU	188	9.421	-17.284	107.682	1.00	51.33	A	C
	ATOM	700	OE1	GLU	188	10.033	-17.060	106.614	1.00	51.74	A	O
	ATOM	701	OE2	GLU	188	8.465	-16.582	108.081	1.00	52.98	A	O
	ATOM	702	C	GLU	188	7.860	-21.182	108.814	1.00	45.35	A	C
15	ATOM	703	O	GLU	188	7.975	-22.407	108.769	1.00	44.56	A	O
	ATOM	704	N	ASP	189	7.385	-20.544	109.879	1.00	44.44	A	N
	ATOM	705	CA	ASP	189	6.945	-21.271	111.062	1.00	43.61	A	C
	ATOM	706	CB	ASP	189	6.674	-20.307	112.215	1.00	44.85	A	C
20	ATOM	707	CG	ASP	189	7.942	-19.883	112.922	1.00	45.63	A	C
	ATOM	708	OD1	ASP	189	7.856	-19.099	113.886	1.00	46.80	A	O
	ATOM	709	OD2	ASP	189	9.027	-20.339	112.513	1.00	47.10	A	O
	ATOM	710	C	ASP	189	5.689	-22.070	110.750	1.00	42.60	A	C
	ATOM	711	O	ASP	189	5.476	-23.142	111.309	1.00	42.20	A	O
25	ATOM	712	N	GLN	190	4.855	-21.541	109.860	1.00	41.71	A	N
	ATOM	713	CA	GLN	190	3.636	-22.230	109.463	1.00	41.03	A	C
	ATOM	714	CB	GLN	190	2.793	-21.346	108.548	1.00	40.62	A	C
	ATOM	715	CG	GLN	190	2.293	-20.072	109.203	1.00	40.82	A	C
	ATOM	716	CD	GLN	190	1.285	-19.330	108.348	1.00	40.63	A	C
30	ATOM	717	OE1	GLN	190	0.993	-18.158	108.590	1.00	41.15	A	O
	ATOM	718	NE2	GLN	190	0.737	-20.012	107.350	1.00	39.87	A	N
	ATOM	719	C	GLN	190	4.005	-23.514	108.733	1.00	40.60	A	C
	ATOM	720	O	GLN	190	3.408	-24.561	108.964	1.00	40.55	A	O
	ATOM	721	N	ILE	191	4.993	-23.422	107.850	1.00	40.63	A	N
35	ATOM	722	CA	ILE	191	5.464	-24.575	107.095	1.00	40.39	A	C
	ATOM	723	CB	ILE	191	6.622	-24.196	106.142	1.00	41.16	A	C
	ATOM	724	CG2	ILE	191	7.032	-25.409	105.325	1.00	41.08	A	C
	ATOM	725	CG1	ILE	191	6.206	-23.050	105.216	1.00	42.55	A	C
	ATOM	726	CD1	ILE	191	5.024	-23.362	104.324	1.00	43.94	A	C
40	ATOM	727	C	ILE	191	5.982	-25.635	108.061	1.00	39.72	A	C
	ATOM	728	O	ILE	191	5.573	-26.792	108.009	1.00	40.14	A	O
	ATOM	729	N	SER	192	6.886	-25.227	108.944	1.00	38.77	A	N
	ATOM	730	CA	SER	192	7.476	-26.135	109.918	1.00	38.58	A	C
	ATOM	731	CB	SER	192	8.433	-25.369	110.836	1.00	39.73	A	C
45	ATOM	732	OG	SER	192	9.405	-24.673	110.072	1.00	41.62	A	O
	ATOM	733	C	SER	192	6.425	-26.850	110.760	1.00	36.86	A	C
	ATOM	734	O	SER	192	6.443	-28.075	110.868	1.00	36.31	A	O
	ATOM	735	N	LEU	193	5.512	-26.087	111.353	1.00	35.10	A	N
	ATOM	736	CA	LEU	193	4.469	-26.675	112.181	1.00	34.68	A	C
50	ATOM	737	CB	LEU	193	3.611	-25.580	112.821	1.00	34.16	A	C
	ATOM	738	CG	LEU	193	4.279	-24.708	113.887	1.00	34.02	A	C
	ATOM	739	CD1	LEU	193	3.258	-23.734	114.445	1.00	33.54	A	C
	ATOM	740	CD2	LEU	193	4.842	-25.581	115.005	1.00	33.52	A	C
	ATOM	741	C	LEU	193	3.582	-27.636	111.395	1.00	34.25	A	C
55	ATOM	742	O	LEU	193	3.222	-28.699	111.888	1.00	32.86	A	O
	ATOM	743	N	LEU	194	3.241	-27.257	110.169	1.00	34.57	A	N
	ATOM	744	CA	LEU	194	2.399	-28.084	109.317	1.00	35.38	A	C
	ATOM	745	CB	LEU	194	2.075	-27.335	108.025	1.00	36.27	A	C
	ATOM	746	CG	LEU	194	0.950	-27.911	107.161	1.00	37.99	A	C

-182-

	ATOM	747	CD1	LEU	194	-0.388	-27.777	107.890	1.00	36.63	A	C
	ATOM	748	CD2	LEU	194	0.906	-27.162	105.833	1.00	39.17	A	C
	ATOM	749	C	LEU	194	3.061	-29.420	108.979	1.00	35.03	A	C
5	ATOM	750	O	LEU	194	2.418	-30.470	109.027	1.00	34.17	A	O
	ATOM	751	N	LYS	195	4.342	-29.376	108.626	1.00	34.97	A	N
	ATOM	752	CA	LYS	195	5.079	-30.587	108.285	1.00	34.93	A	C
	ATOM	753	CB	LYS	195	6.491	-30.241	107.796	1.00	36.64	A	C
	ATOM	754	CG	LYS	195	6.542	-29.420	106.513	1.00	38.77	A	C
10	ATOM	755	CD	LYS	195	7.978	-29.272	106.017	1.00	40.24	A	C
	ATOM	756	CE	LYS	195	8.054	-28.509	104.698	1.00	40.73	A	C
	ATOM	757	NZ	LYS	195	7.263	-29.167	103.615	1.00	42.42	A	N
	ATOM	758	C	LYS	195	5.190	-31.510	109.493	1.00	33.81	A	C
	ATOM	759	O	LYS	195	5.027	-32.729	109.382	1.00	33.63	A	O
15	ATOM	760	N	GLY	196	5.465	-30.921	110.650	1.00	32.20	A	N
	ATOM	761	CA	GLY	196	5.617	-31.713	111.852	1.00	30.60	A	C
	ATOM	762	C	GLY	196	4.346	-32.292	112.443	1.00	29.37	A	C
	ATOM	763	O	GLY	196	4.400	-33.342	113.085	1.00	28.60	A	O
	ATOM	764	N	ALA	197	3.202	-31.648	112.210	1.00	27.66	A	N
20	ATOM	765	CA	ALA	197	1.958	-32.119	112.804	1.00	26.31	A	C
	ATOM	766	CB	ALA	197	1.400	-31.028	113.699	1.00	26.25	A	C
	ATOM	767	C	ALA	197	0.836	-32.666	111.919	1.00	25.33	A	C
	ATOM	768	O	ALA	197	-0.058	-33.329	112.427	1.00	24.11	A	O
	ATOM	769	N	ALA	198	0.869	-32.396	110.617	1.00	24.59	A	N
25	ATOM	770	CA	ALA	198	-0.188	-32.860	109.702	1.00	23.71	A	C
	ATOM	771	CB	ALA	198	0.250	-32.663	108.248	1.00	21.84	A	C
	ATOM	772	C	ALA	198	-0.656	-34.307	109.901	1.00	22.64	A	C
	ATOM	773	O	ALA	198	-1.838	-34.554	110.102	1.00	22.27	A	O
	ATOM	774	N	VAL	199	0.267	-35.259	109.825	1.00	21.45	A	N
30	ATOM	775	CA	VAL	199	-0.081	-36.664	109.988	1.00	20.82	A	C
	ATOM	776	CB	VAL	199	1.132	-37.567	109.682	1.00	20.86	A	C
	ATOM	777	CG1	VAL	199	0.811	-39.020	110.025	1.00	20.51	A	C
	ATOM	778	CG2	VAL	199	1.496	-37.441	108.201	1.00	19.73	A	C
	ATOM	779	C	VAL	199	-0.616	-36.961	111.387	1.00	21.29	A	C
35	ATOM	780	O	VAL	199	-1.569	-37.724	111.539	1.00	20.92	A	O
	ATOM	781	N	GLU	200	-0.012	-36.353	112.406	1.00	20.35	A	N
	ATOM	782	CA	GLU	200	-0.463	-36.549	113.775	1.00	21.19	A	C
	ATOM	783	CB	GLU	200	0.444	-35.780	114.747	1.00	21.68	A	C
	ATOM	784	CG	GLU	200	1.844	-36.367	114.891	1.00	22.67	A	C
40	ATOM	785	CD	GLU	200	2.713	-35.615	115.895	1.00	23.90	A	C
	ATOM	786	OE1	GLU	200	2.179	-34.813	116.690	1.00	23.20	A	O
	ATOM	787	OE2	GLU	200	3.941	-35.845	115.897	1.00	25.78	A	O
	ATOM	788	C	GLU	200	-1.919	-36.082	113.930	1.00	21.10	A	C
	ATOM	789	O	GLU	200	-2.766	-36.802	114.466	1.00	20.46	A	O
45	ATOM	790	N	ILE	201	-2.200	-34.872	113.459	1.00	20.78	A	N
	ATOM	791	CA	ILE	201	-3.543	-34.310	113.531	1.00	21.26	A	C
	ATOM	792	CB	ILE	201	-3.593	-32.896	112.901	1.00	21.50	A	C
	ATOM	793	CG2	ILE	201	-5.042	-32.407	112.825	1.00	22.57	A	C
	ATOM	794	CG1	ILE	201	-2.753	-31.919	113.735	1.00	21.48	A	C
50	ATOM	795	CD1	ILE	201	-2.661	-30.520	113.133	1.00	21.35	A	C
	ATOM	796	C	ILE	201	-4.540	-35.209	112.806	1.00	21.13	A	C
	ATOM	797	O	ILE	201	-5.659	-35.413	113.278	1.00	21.64	A	O
	ATOM	798	N	CYS	202	-4.136	-35.737	111.657	1.00	20.20	A	N
	ATOM	799	CA	CYS	202	-5.007	-36.617	110.893	1.00	20.37	A	C
55	ATOM	800	CB	CYS	202	-4.332	-37.024	109.585	1.00	20.42	A	C
	ATOM	801	SG	CYS	202	-4.259	-35.662	108.393	1.00	21.08	A	S
	ATOM	802	C	CYS	202	-5.413	-37.848	111.694	1.00	18.85	A	C
	ATOM	803	O	CYS	202	-6.582	-38.234	111.687	1.00	18.40	A	O
	ATOM	804	N	HIS	203	-4.461	-38.465	112.384	1.00	18.00	A	N

-183-

	ATOM	805	CA	HIS	203	-4.781	-39.635	113.190	1.00	18.29	A	C
	ATOM	806	CB	HIS	203	-3.505	-40.312	113.686	1.00	17.63	A	C
	ATOM	807	CG	HIS	203	-2.837	-41.157	112.646	1.00	18.10	A	C
	ATOM	808	CD2	HIS	203	-1.678	-40.986	111.967	1.00	17.36	A	C
5	ATOM	809	ND1	HIS	203	-3.398	-42.318	112.161	1.00	17.64	A	N
	ATOM	810	CE1	HIS	203	-2.616	-42.825	111.225	1.00	17.59	A	C
	ATOM	811	NE2	HIS	203	-1.567	-42.035	111.087	1.00	17.70	A	N
	ATOM	812	C	HIS	203	-5.690	-39.255	114.361	1.00	18.57	A	C
10	ATOM	813	O	HIS	203	-6.586	-40.012	114.724	1.00	17.74	A	O
	ATOM	814	N	ILE	204	-5.470	-38.080	114.945	1.00	17.95	A	N
	ATOM	815	CA	ILE	204	-6.326	-37.634	116.031	1.00	18.97	A	C
	ATOM	816	CB	ILE	204	-5.867	-36.271	116.595	1.00	18.95	A	C
	ATOM	817	CG2	ILE	204	-6.949	-35.696	117.530	1.00	17.63	A	C
	ATOM	818	CG1	ILE	204	-4.529	-36.436	117.322	1.00	17.08	A	C
15	ATOM	819	CD1	ILE	204	-3.990	-35.142	117.913	1.00	16.88	A	C
	ATOM	820	C	ILE	204	-7.754	-37.491	115.490	1.00	19.25	A	C
	ATOM	821	O	ILE	204	-8.708	-37.949	116.111	1.00	19.34	A	O
	ATOM	822	N	VAL	205	-7.890	-36.859	114.327	1.00	19.23	A	N
20	ATOM	823	CA	VAL	205	-9.195	-36.660	113.708	1.00	19.58	A	C
	ATOM	824	CB	VAL	205	-9.070	-35.782	112.437	1.00	19.63	A	C
	ATOM	825	CG1	VAL	205	-10.396	-35.756	111.680	1.00	20.05	A	C
	ATOM	826	CG2	VAL	205	-8.666	-34.371	112.823	1.00	19.24	A	C
	ATOM	827	C	VAL	205	-9.881	-37.979	113.330	1.00	19.64	A	C
	ATOM	828	O	VAL	205	-11.078	-38.145	113.545	1.00	19.82	A	O
25	ATOM	829	N	LEU	206	-9.112	-38.911	112.773	1.00	19.63	A	N
	ATOM	830	CA	LEU	206	-9.639	-40.204	112.342	1.00	19.49	A	C
	ATOM	831	CB	LEU	206	-8.650	-40.866	111.379	1.00	19.58	A	C
	ATOM	832	CG	LEU	206	-8.980	-40.934	109.879	1.00	21.14	A	C
	ATOM	833	CD1	LEU	206	-9.924	-39.817	109.455	1.00	20.56	A	C
30	ATOM	834	CD2	LEU	206	-7.674	-40.869	109.094	1.00	20.01	A	C
	ATOM	835	C	LEU	206	-9.977	-41.175	113.469	1.00	18.64	A	C
	ATOM	836	O	LEU	206	-10.662	-42.178	113.242	1.00	18.00	A	O
	ATOM	837	N	ASN	207	-9.515	-40.877	114.678	1.00	17.72	A	N
	ATOM	838	CA	ASN	207	-9.763	-41.752	115.817	1.00	17.71	A	C
35	ATOM	839	CB	ASN	207	-9.148	-41.162	117.089	1.00	16.46	A	C
	ATOM	840	CG	ASN	207	-9.297	-42.086	118.291	1.00	17.11	A	C
	ATOM	841	OD1	ASN	207	-10.037	-41.792	119.233	1.00	16.94	A	O
	ATOM	842	ND2	ASN	207	-8.600	-43.216	118.255	1.00	14.15	A	N
	ATOM	843	C	ASN	207	-11.247	-42.043	116.052	1.00	18.08	A	C
40	ATOM	844	O	ASN	207	-11.601	-43.148	116.479	1.00	17.24	A	O
	ATOM	845	N	THR	208	-12.117	-41.069	115.782	1.00	17.73	A	N
	ATOM	846	CA	THR	208	-13.542	-41.306	115.978	1.00	19.30	A	C
	ATOM	847	CB	THR	208	-14.377	-40.000	115.973	1.00	19.32	A	C
	ATOM	848	OG1	THR	208	-13.996	-39.163	114.875	1.00	20.78	A	O
45	ATOM	849	CG2	THR	208	-14.184	-39.262	117.284	1.00	20.86	A	C
	ATOM	850	C	THR	208	-14.145	-42.306	114.987	1.00	19.41	A	C
	ATOM	851	O	THR	208	-15.288	-42.716	115.150	1.00	19.80	A	O
	ATOM	852	N	THR	209	-13.394	-42.706	113.964	1.00	19.05	A	N
	ATOM	853	CA	THR	209	-13.909	-43.722	113.045	1.00	19.58	A	C
50	ATOM	854	CB	THR	209	-13.389	-43.556	111.608	1.00	19.77	A	C
	ATOM	855	OG1	THR	209	-11.978	-43.799	111.584	1.00	19.93	A	O
	ATOM	856	CG2	THR	209	-13.688	-42.146	111.073	1.00	20.26	A	C
	ATOM	857	C	THR	209	-13.456	-45.103	113.537	1.00	19.57	A	C
	ATOM	858	O	THR	209	-13.954	-46.128	113.079	1.00	19.72	A	O
55	ATOM	859	N	PHE	210	-12.520	-45.127	114.483	1.00	19.02	A	N
	ATOM	860	CA	PHE	210	-12.000	-46.386	115.006	1.00	20.29	A	C
	ATOM	861	CB	PHE	210	-10.765	-46.127	115.873	1.00	19.30	A	C
	ATOM	862	CG	PHE	210	-9.938	-47.354	116.129	1.00	19.82	A	C

-184-

5	ATOM	863	CD1	PHE	210	-9.215	-47.948	115.096	1.00	19.46	A	C
	ATOM	864	CD2	PHE	210	-9.891	-47.926	117.399	1.00	18.74	A	C
	ATOM	865	CE1	PHE	210	-8.454	-49.096	115.325	1.00	19.60	A	C
	ATOM	866	CE2	PHE	210	-9.135	-49.072	117.641	1.00	19.21	A	C
	ATOM	867	CZ	PHE	210	-8.415	-49.661	116.605	1.00	19.22	A	C
10	ATOM	868	C	PHE	210	-13.035	-47.176	115.810	1.00	21.23	A	C
	ATOM	869	O	PHE	210	-13.639	-46.667	116.756	1.00	20.44	A	O
	ATOM	870	N	CYS	211	-13.229	-48.430	115.421	1.00	22.24	A	N
	ATOM	871	CA	CYS	211	-14.175	-49.304	116.087	1.00	24.03	A	C
	ATOM	872	CB	CYS	211	-14.950	-50.117	115.049	1.00	24.67	A	C
15	ATOM	873	SG	CYS	211	-16.182	-51.252	115.747	1.00	25.21	A	S
	ATOM	874	C	CYS	211	-13.385	-50.228	117.006	1.00	24.78	A	C
	ATOM	875	O	CYS	211	-12.508	-50.962	116.562	1.00	23.56	A	O
	ATOM	876	N	LEU	212	-13.690	-50.179	118.294	1.00	25.72	A	N
	ATOM	877	CA	LEU	212	-12.989	-51.006	119.262	1.00	27.59	A	C
20	ATOM	878	CB	LEU	212	-13.380	-50.578	120.671	1.00	27.74	A	C
	ATOM	879	CG	LEU	212	-12.881	-49.185	121.058	1.00	28.59	A	C
	ATOM	880	CD1	LEU	212	-13.486	-48.759	122.396	1.00	28.93	A	C
	ATOM	881	CD2	LEU	212	-11.365	-49.210	121.125	1.00	27.26	A	C
	ATOM	882	C	LEU	212	-13.272	-52.489	119.075	1.00	29.09	A	C
25	ATOM	883	O	LEU	212	-12.374	-53.322	119.189	1.00	28.72	A	O
	ATOM	884	N	GLN	213	-14.524	-52.805	118.765	1.00	30.49	A	N
	ATOM	885	CA	GLN	213	-14.956	-54.181	118.583	1.00	32.47	A	C
	ATOM	886	CB	GLN	213	-16.457	-54.204	118.283	1.00	35.49	A	C
	ATOM	887	CG	GLN	213	-17.157	-55.523	118.581	1.00	40.38	A	C
30	ATOM	888	CD	GLN	213	-17.315	-55.780	120.073	1.00	42.74	A	C
	ATOM	889	OE1	GLN	213	-17.855	-54.945	120.806	1.00	44.72	A	O
	ATOM	890	NE2	GLN	213	-16.849	-56.939	120.528	1.00	44.13	A	N
	ATOM	891	C	GLN	213	-14.200	-54.911	117.474	1.00	31.71	A	C
	ATOM	892	O	GLN	213	-13.745	-56.034	117.662	1.00	31.33	A	O
35	ATOM	893	N	THR	214	-14.068	-54.272	116.319	1.00	30.92	A	N
	ATOM	894	CA	THR	214	-13.388	-54.888	115.183	1.00	30.21	A	C
	ATOM	895	CB	THR	214	-14.189	-54.681	113.898	1.00	30.65	A	C
	ATOM	896	OG1	THR	214	-14.410	-53.278	113.707	1.00	30.08	A	O
	ATOM	897	CG2	THR	214	-15.528	-55.404	113.983	1.00	30.64	A	C
40	ATOM	898	C	THR	214	-11.971	-54.390	114.922	1.00	29.58	A	C
	ATOM	899	O	THR	214	-11.272	-54.943	114.079	1.00	29.04	A	O
	ATOM	900	N	GLN	215	-11.555	-53.341	115.625	1.00	29.13	A	N
	ATOM	901	CA	GLN	215	-10.214	-52.788	115.454	1.00	29.85	A	C
	ATOM	902	CB	GLN	215	-9.179	-53.869	115.775	1.00	31.30	A	C
45	ATOM	903	CG	GLN	215	-7.916	-53.384	116.476	1.00	35.10	A	C
	ATOM	904	CD	GLN	215	-8.150	-52.959	117.919	1.00	36.36	A	C
	ATOM	905	OE1	GLN	215	-9.137	-53.351	118.547	1.00	36.52	A	O
	ATOM	906	NE2	GLN	215	-7.228	-52.163	118.456	1.00	37.92	A	N
	ATOM	907	C	GLN	215	-10.045	-52.300	114.007	1.00	29.28	A	C
50	ATOM	908	O	GLN	215	-8.980	-52.457	113.397	1.00	29.33	A	O
	ATOM	909	N	ASN	216	-11.110	-51.715	113.472	1.00	27.92	A	N
	ATOM	910	CA	ASN	216	-11.138	-51.208	112.104	1.00	27.75	A	C
	ATOM	911	CB	ASN	216	-12.198	-51.953	111.276	1.00	29.04	A	C
	ATOM	912	CG	ASN	216	-11.820	-53.388	110.966	1.00	31.13	A	C
55	ATOM	913	OD1	ASN	216	-12.672	-54.183	110.566	1.00	31.15	A	O
	ATOM	914	ND2	ASN	216	-10.544	-53.728	111.130	1.00	32.04	A	N
	ATOM	915	C	ASN	216	-11.521	-49.739	112.109	1.00	26.04	A	C
	ATOM	916	O	ASN	216	-12.077	-49.236	113.079	1.00	25.94	A	O
	ATOM	917	N	PHE	217	-11.226	-49.057	111.012	1.00	24.54	A	N
	ATOM	918	CA	PHE	217	-11.607	-47.660	110.868	1.00	23.68	A	C
	ATOM	919	CB	PHE	217	-10.474	-46.846	110.247	1.00	21.91	A	C
	ATOM	920	CG	PHE	217	-9.271	-46.723	111.132	1.00	21.44	A	C

-185-

	ATOM	921	CD1	PHE	217	-8.295	-47.709	111.143	1.00	20.23	A	C
	ATOM	922	CD2	PHE	217	-9.127	-45.625	111.977	1.00	21.42	A	C
	ATOM	923	CE1	PHE	217	-7.191	-47.603	111.982	1.00	21.65	A	C
5	ATOM	924	CE2	PHE	217	-8.024	-45.509	112.825	1.00	21.20	A	C
	ATOM	925	CZ	PHE	217	-7.057	-46.497	112.826	1.00	20.69	A	C
	ATOM	926	C	PHE	217	-12.821	-47.677	109.944	1.00	23.24	A	C
	ATOM	927	O	PHE	217	-12.714	-48.053	108.778	1.00	23.15	A	O
	ATOM	928	N	LEU	218	-13.976	-47.292	110.475	1.00	22.85	A	N
10	ATOM	929	CA	LEU	218	-15.217	-47.292	109.697	1.00	22.28	A	C
	ATOM	930	CB	LEU	218	-16.388	-47.702	110.591	1.00	22.69	A	C
	ATOM	931	CG	LEU	218	-16.185	-49.017	111.344	1.00	24.13	A	C
	ATOM	932	CD1	LEU	218	-17.413	-49.316	112.191	1.00	24.57	A	C
	ATOM	933	CD2	LEU	218	-15.923	-50.148	110.346	1.00	24.80	A	C
15	ATOM	934	C	LEU	218	-15.478	-45.919	109.110	1.00	21.34	A	C
	ATOM	935	O	LEU	218	-15.830	-44.984	109.830	1.00	20.56	A	O
	ATOM	936	N	CYS	219	-15.305	-45.805	107.798	1.00	21.05	A	N
	ATOM	937	CA	CYS	219	-15.502	-44.541	107.101	1.00	20.80	A	C
	ATOM	938	CB	CYS	219	-14.203	-44.136	106.399	1.00	20.03	A	C
20	ATOM	939	SG	CYS	219	-12.762	-44.055	107.502	1.00	21.17	A	S
	ATOM	940	C	CYS	219	-16.640	-44.667	106.087	1.00	21.14	A	C
	ATOM	941	O	CYS	219	-16.414	-44.904	104.889	1.00	20.85	A	O
	ATOM	942	N	GLY	220	-17.865	-44.492	106.574	1.00	21.18	A	N
	ATOM	943	CA	GLY	220	-19.024	-44.612	105.710	1.00	21.35	A	C
25	ATOM	944	C	GLY	220	-19.104	-46.047	105.222	1.00	21.61	A	C
	ATOM	945	O	GLY	220	-19.079	-46.971	106.025	1.00	21.96	A	O
	ATOM	946	N	PRO	221	-19.197	-46.270	103.908	1.00	21.46	A	N
	ATOM	947	CD	PRO	221	-19.369	-45.295	102.816	1.00	21.21	A	C
	ATOM	948	CA	PRO	221	-19.273	-47.640	103.402	1.00	22.15	A	C
30	ATOM	949	CB	PRO	221	-19.909	-47.451	102.027	1.00	21.42	A	C
	ATOM	950	CG	PRO	221	-19.277	-46.164	101.576	1.00	20.84	A	C
	ATOM	951	C	PRO	221	-17.893	-48.313	103.320	1.00	22.19	A	C
	ATOM	952	O	PRO	221	-17.794	-49.481	102.938	1.00	22.79	A	O
	ATOM	953	N	LEU	222	-16.841	-47.577	103.678	1.00	21.79	A	N
35	ATOM	954	CA	LEU	222	-15.473	-48.097	103.633	1.00	21.31	A	C
	ATOM	955	CB	LEU	222	-14.511	-47.032	103.093	1.00	19.09	A	C
	ATOM	956	CG	LEU	222	-14.746	-46.584	101.644	1.00	18.95	A	C
	ATOM	957	CD1	LEU	222	-13.870	-45.392	101.319	1.00	18.64	A	C
	ATOM	958	CD2	LEU	222	-14.460	-47.738	100.691	1.00	16.82	A	C
40	ATOM	959	C	LEU	222	-14.985	-48.569	104.999	1.00	21.86	A	C
	ATOM	960	O	LEU	222	-15.313	-47.974	106.030	1.00	21.48	A	O
	ATOM	961	N	ARG	223	-14.184	-49.634	104.979	1.00	21.57	A	N
	ATOM	962	CA	ARG	223	-13.618	-50.249	106.175	1.00	22.37	A	C
	ATOM	963	CB	ARG	223	-14.377	-51.558	106.465	1.00	24.98	A	C
45	ATOM	964	CG	ARG	223	-13.739	-52.476	107.490	1.00	28.92	A	C
	ATOM	965	CD	ARG	223	-13.141	-53.746	106.858	1.00	32.82	A	C
	ATOM	966	NE	ARG	223	-14.154	-54.668	106.324	1.00	36.01	A	N
	ATOM	967	CZ	ARG	223	-14.568	-54.692	105.057	1.00	36.66	A	C
	ATOM	968	NH1	ARG	223	-14.058	-53.847	104.167	1.00	36.15	A	N
	ATOM	969	NH2	ARG	223	-15.495	-55.565	104.677	1.00	36.63	A	N
50	ATOM	970	C	ARG	223	-12.113	-50.515	105.967	1.00	21.18	A	C
	ATOM	971	O	ARG	223	-11.718	-51.260	105.070	1.00	20.16	A	O
	ATOM	972	N	TYR	224	-11.277	-49.884	106.782	1.00	18.92	A	N
	ATOM	973	CA	TYR	224	-9.829	-50.070	106.678	1.00	19.29	A	C
55	ATOM	974	CB	TYR	224	-9.088	-48.723	106.716	1.00	17.44	A	C
	ATOM	975	CG	TYR	224	-9.470	-47.770	105.604	1.00	17.07	A	C
	ATOM	976	CD1	TYR	224	-10.560	-46.908	105.741	1.00	16.45	A	C
	ATOM	977	CE1	TYR	224	-10.936	-46.053	104.711	1.00	16.85	A	C
	ATOM	978	CD2	TYR	224	-8.761	-47.751	104.402	1.00	16.10	A	C

-186-

	ATOM	979	CE2	TYR	224	-9.131	-46.897	103.357	1.00	16.65	A	C
	ATOM	980	CZ	TYR	224	-10.225	-46.052	103.521	1.00	16.90	A	C
	ATOM	981	OH	TYR	224	-10.636	-45.234	102.490	1.00	16.57	A	O
5	ATOM	982	C	TYR	224	-9.354	-50.949	107.836	1.00	18.68	A	C
	ATOM	983	O	TYR	224	-9.712	-50.713	108.986	1.00	18.12	A	O
	ATOM	984	N	THR	225	-8.543	-51.951	107.516	1.00	17.86	A	N
	ATOM	985	CA	THR	225	-8.029	-52.894	108.505	1.00	18.12	A	C
	ATOM	986	CB	THR	225	-8.322	-54.355	108.091	1.00	16.87	A	C
10	ATOM	987	OG1	THR	225	-7.612	-54.637	106.883	1.00	16.75	A	O
	ATOM	988	CG2	THR	225	-9.803	-54.578	107.848	1.00	15.99	A	C
	ATOM	989	C	THR	225	-6.514	-52.781	108.624	1.00	17.74	A	C
	ATOM	990	O	THR	225	-5.855	-52.164	107.785	1.00	17.42	A	O
	ATOM	991	N	ILE	226	-5.964	-53.404	109.660	1.00	16.95	A	N
15	ATOM	992	CA	ILE	226	-4.526	-53.390	109.861	1.00	17.61	A	C
	ATOM	993	CB	ILE	226	-4.161	-53.985	111.246	1.00	17.39	A	C
	ATOM	994	CG2	ILE	226	-4.492	-55.476	111.290	1.00	15.65	A	C
	ATOM	995	CG1	ILE	226	-2.685	-53.713	111.555	1.00	17.84	A	C
	ATOM	996	CD1	ILE	226	-2.309	-54.002	112.989	1.00	18.23	A	C
20	ATOM	997	C	ILE	226	-3.823	-54.153	108.714	1.00	17.93	A	C
	ATOM	998	O	ILE	226	-2.662	-53.874	108.403	1.00	16.65	A	O
	ATOM	999	N	GLU	227	-4.530	-55.089	108.072	1.00	17.96	A	N
	ATOM	1000	CA	GLU	227	-3.962	-55.840	106.949	1.00	19.11	A	C
	ATOM	1001	CB	GLU	227	-4.891	-56.981	106.503	1.00	20.72	A	C
25	ATOM	1002	CG	GLU	227	-4.912	-58.231	107.401	1.00	20.80	A	C
	ATOM	1003	CD	GLU	227	-5.526	-57.975	108.761	1.00	21.93	A	C
	ATOM	1004	OE1	GLU	227	-6.513	-57.220	108.833	1.00	23.31	A	O
	ATOM	1005	OE2	GLU	227	-5.040	-58.536	109.760	1.00	21.48	A	O
	ATOM	1006	C	GLU	227	-3.718	-54.914	105.757	1.00	19.73	A	C
30	ATOM	1007	O	GLU	227	-2.805	-55.147	104.954	1.00	18.85	A	O
	ATOM	1008	N	ASP	228	-4.546	-53.877	105.623	1.00	18.55	A	N
	ATOM	1009	CA	ASP	228	-4.371	-52.928	104.533	1.00	19.17	A	C
	ATOM	1010	CB	ASP	228	-5.504	-51.886	104.522	1.00	19.08	A	C
	ATOM	1011	CG	ASP	228	-6.846	-52.496	104.159	1.00	19.07	A	C
35	ATOM	1012	OD1	ASP	228	-6.873	-53.316	103.219	1.00	20.93	A	O
	ATOM	1013	OD2	ASP	228	-7.869	-52.164	104.795	1.00	18.63	A	O
	ATOM	1014	C	ASP	228	-3.012	-52.251	104.691	1.00	18.73	A	C
	ATOM	1015	O	ASP	228	-2.279	-52.077	103.715	1.00	19.17	A	O
	ATOM	1016	N	GLY	229	-2.672	-51.879	105.922	1.00	18.10	A	N
40	ATOM	1017	CA	GLY	229	-1.386	-51.253	106.164	1.00	17.50	A	C
	ATOM	1018	C	GLY	229	-0.245	-52.236	105.926	1.00	17.22	A	C
	ATOM	1019	O	GLY	229	0.771	-51.898	105.321	1.00	15.48	A	O
	ATOM	1020	N	ALA	230	-0.413	-53.461	106.410	1.00	17.33	A	N
	ATOM	1021	CA	ALA	230	0.608	-54.485	106.247	1.00	18.15	A	C
45	ATOM	1022	CB	ALA	230	0.195	-55.745	106.987	1.00	16.66	A	C
	ATOM	1023	C	ALA	230	0.855	-54.795	104.770	1.00	19.00	A	C
	ATOM	1024	O	ALA	230	2.001	-54.934	104.344	1.00	19.76	A	O
	ATOM	1025	N	ARG	231	-0.219	-54.887	103.990	1.00	19.49	A	N
	ATOM	1026	CA	ARG	231	-0.109	-55.193	102.566	1.00	19.81	A	C
50	ATOM	1027	CB	ARG	231	-1.491	-55.499	101.973	1.00	20.78	A	C
	ATOM	1028	CG	ARG	231	-2.159	-56.765	102.524	1.00	22.44	A	C
	ATOM	1029	CD	ARG	231	-1.366	-58.040	102.205	1.00	24.31	A	C
	ATOM	1030	NE	ARG	231	-1.373	-58.385	100.783	1.00	26.32	A	N
	ATOM	1031	CZ	ARG	231	-2.383	-58.974	100.143	1.00	28.16	A	C
55	ATOM	1032	NH1	ARG	231	-3.498	-59.305	100.780	1.00	27.73	A	N
	ATOM	1033	NH2	ARG	231	-2.276	-59.233	98.846	1.00	30.42	A	N
	ATOM	1034	C	ARG	231	0.590	-54.127	101.721	1.00	19.74	A	C
	ATOM	1035	O	ARG	231	1.107	-54.451	100.650	1.00	20.20	A	O
	ATOM	1036	N	VAL	232	0.608	-52.867	102.170	1.00	18.61	A	N

-187-

	ATOM	1037	CA	VAL	232	1.296	-51.826	101.404	1.00	17.26	A	C
	ATOM	1038	CB	VAL	232	0.569	-50.434	101.462	1.00	17.52	A	C
	ATOM	1039	CG1	VAL	232	-0.855	-50.569	100.919	1.00	17.25	A	C
5	ATOM	1040	CG2	VAL	232	0.563	-49.875	102.879	1.00	16.49	A	C
	ATOM	1041	C	VAL	232	2.748	-51.670	101.852	1.00	17.95	A	C
	ATOM	1042	O	VAL	232	3.469	-50.800	101.358	1.00	17.18	A	O
	ATOM	1043	N	GLY	233	3.189	-52.510	102.788	1.00	18.73	A	N
	ATOM	1044	CA	GLY	233	4.582	-52.442	103.205	1.00	19.65	A	C
10	ATOM	1045	C	GLY	233	4.955	-51.997	104.608	1.00	20.28	A	C
	ATOM	1046	O	GLY	233	6.129	-52.078	104.969	1.00	20.44	A	O
	ATOM	1047	N	PHE	234	3.999	-51.514	105.397	1.00	19.59	A	N
	ATOM	1048	CA	PHE	234	4.313	-51.107	106.764	1.00	20.47	A	C
	ATOM	1049	CB	PHE	234	3.134	-50.366	107.401	1.00	20.71	A	C
15	ATOM	1050	CG	PHE	234	2.949	-48.963	106.901	1.00	21.67	A	C
	ATOM	1051	CD1	PHE	234	1.790	-48.602	106.229	1.00	21.54	A	C
	ATOM	1052	CD2	PHE	234	3.922	-47.996	107.133	1.00	22.13	A	C
	ATOM	1053	CE1	PHE	234	1.596	-47.291	105.794	1.00	23.35	A	C
	ATOM	1054	CE2	PHE	234	3.741	-46.681	106.703	1.00	23.24	A	C
20	ATOM	1055	CZ	PHE	234	2.572	-46.328	106.032	1.00	22.54	A	C
	ATOM	1056	C	PHE	234	4.648	-52.322	107.633	1.00	20.13	A	C
	ATOM	1057	O	PHE	234	4.039	-53.388	107.503	1.00	19.24	A	O
	ATOM	1058	N	GLN	235	5.606	-52.153	108.534	1.00	20.97	A	N
	ATOM	1059	CA	GLN	235	5.997	-53.231	109.427	1.00	22.42	A	C
25	ATOM	1060	CB	GLN	235	7.348	-52.917	110.064	1.00	24.45	A	C
	ATOM	1061	CG	GLN	235	8.493	-52.968	109.069	1.00	27.92	A	C
	ATOM	1062	CD	GLN	235	9.841	-52.727	109.709	1.00	30.93	A	C
	ATOM	1063	OE1	GLN	235	10.843	-53.322	109.304	1.00	33.56	A	O
	ATOM	1064	NE2	GLN	235	9.883	-51.847	110.703	1.00	30.93	A	N
30	ATOM	1065	C	GLN	235	4.932	-53.444	110.494	1.00	21.69	A	C
	ATOM	1066	O	GLN	235	4.303	-52.498	110.966	1.00	20.35	A	O
	ATOM	1067	N	VAL	236	4.729	-54.702	110.863	1.00	21.75	A	N
	ATOM	1068	CA	VAL	236	3.725	-55.064	111.850	1.00	20.74	A	C
	ATOM	1069	CB	VAL	236	3.679	-56.585	112.035	1.00	20.71	A	C
35	ATOM	1070	CG1	VAL	236	2.728	-56.953	113.178	1.00	19.30	A	C
	ATOM	1071	CG2	VAL	236	3.233	-57.231	110.730	1.00	20.83	A	C
	ATOM	1072	C	VAL	236	3.906	-54.393	113.197	1.00	21.19	A	C
	ATOM	1073	O	VAL	236	2.933	-53.928	113.785	1.00	20.57	A	O
	ATOM	1074	N	GLU	237	5.138	-54.346	113.695	1.00	21.62	A	N
40	ATOM	1075	CA	GLU	237	5.400	-53.702	114.981	1.00	23.17	A	C
	ATOM	1076	CB	GLU	237	6.890	-53.788	115.323	1.00	25.38	A	C
	ATOM	1077	CG	GLU	237	7.309	-52.979	116.535	1.00	29.56	A	C
	ATOM	1078	CD	GLU	237	8.719	-53.315	117.002	1.00	32.34	A	C
	ATOM	1079	OE1	GLU	237	9.616	-53.489	116.146	1.00	34.48	A	O
45	ATOM	1080	OE2	GLU	237	8.931	-53.400	118.227	1.00	33.42	A	O
	ATOM	1081	C	GLU	237	4.940	-52.241	114.945	1.00	22.30	A	C
	ATOM	1082	O	GLU	237	4.354	-51.745	115.905	1.00	21.24	A	O
	ATOM	1083	N	PHE	238	5.210	-51.558	113.836	1.00	21.77	A	N
	ATOM	1084	CA	PHE	238	4.779	-50.169	113.667	1.00	22.10	A	C
50	ATOM	1085	CB	PHE	238	5.284	-49.611	112.331	1.00	21.91	A	C
	ATOM	1086	CG	PHE	238	4.661	-48.296	111.954	1.00	22.44	A	C
	ATOM	1087	CD1	PHE	238	5.015	-47.123	112.622	1.00	22.09	A	C
	ATOM	1088	CD2	PHE	238	3.687	-48.234	110.961	1.00	22.65	A	C
	ATOM	1089	CE1	PHE	238	4.409	-45.914	112.310	1.00	21.36	A	C
55	ATOM	1090	CE2	PHE	238	3.073	-47.026	110.636	1.00	22.78	A	C
	ATOM	1091	CZ	PHE	238	3.436	-45.861	111.316	1.00	22.50	A	C
	ATOM	1092	C	PHE	238	3.245	-50.142	113.673	1.00	21.89	A	C
	ATOM	1093	O	PHE	238	2.618	-49.354	114.378	1.00	20.84	A	O
	ATOM	1094	N	LEU	239	2.653	-51.013	112.863	1.00	22.09	A	N

-188-

5	ATOM	1095	CA	LEU	239	1.205	-51.118	112.759	1.00	22.46	A	C
	ATOM	1096	CB	LEU	239	0.845	-52.241	111.778	1.00	21.56	A	C
	ATOM	1097	CG	LEU	239	0.402	-51.905	110.343	1.00	23.54	A	C
	ATOM	1098	CD1	LEU	239	0.860	-50.519	109.926	1.00	22.90	A	C
	ATOM	1099	CD2	LEU	239	0.925	-52.977	109.388	1.00	21.20	A	C
10	ATOM	1100	C	LEU	239	0.577	-51.376	114.132	1.00	22.41	A	C
	ATOM	1101	O	LEU	239	-0.441	-50.776	114.470	1.00	21.62	A	O
	ATOM	1102	N	GLU	240	1.182	-52.262	114.923	1.00	22.26	A	N
	ATOM	1103	CA	GLU	240	0.668	-52.563	116.256	1.00	22.89	A	C
	ATOM	1104	CB	GLU	240	1.471	-53.690	116.918	1.00	25.34	A	C
15	ATOM	1105	CG	GLU	240	1.267	-55.069	116.305	1.00	29.77	A	C
	ATOM	1106	CD	GLU	240	-0.189	-55.498	116.294	1.00	33.75	A	C
	ATOM	1107	OE1	GLU	240	-1.022	-54.811	116.927	1.00	36.81	A	O
	ATOM	1108	OE2	GLU	240	-0.507	-56.527	115.658	1.00	35.46	A	O
	ATOM	1109	C	GLU	240	0.705	-51.327	117.151	1.00	21.32	A	C
20	ATOM	1110	O	GLU	240	-0.224	-51.081	117.906	1.00	20.62	A	O
	ATOM	1111	N	LEU	241	1.780	-50.554	117.070	1.00	20.96	A	N
	ATOM	1112	CA	LEU	241	1.888	-49.349	117.883	1.00	22.45	A	C
	ATOM	1113	CB	LEU	241	3.239	-48.664	117.648	1.00	24.05	A	C
	ATOM	1114	CG	LEU	241	3.466	-47.321	118.363	1.00	26.05	A	C
25	ATOM	1115	CD1	LEU	241	3.433	-47.531	119.877	1.00	27.21	A	C
	ATOM	1116	CD2	LEU	241	4.806	-46.727	117.945	1.00	26.89	A	C
	ATOM	1117	C	LEU	241	0.757	-48.389	117.511	1.00	21.92	A	C
	ATOM	1118	O	LEU	241	0.067	-47.855	118.381	1.00	21.86	A	O
	ATOM	1119	N	LEU	242	0.572	-48.194	116.210	1.00	20.84	A	N
30	ATOM	1120	CA	LEU	242	-0.452	-47.303	115.677	1.00	20.79	A	C
	ATOM	1121	CB	LEU	242	-0.433	-47.341	114.146	1.00	19.93	A	C
	ATOM	1122	CG	LEU	242	-0.682	-46.031	113.392	1.00	21.77	A	C
	ATOM	1123	CD1	LEU	242	-1.129	-46.358	111.984	1.00	19.10	A	C
	ATOM	1124	CD2	LEU	242	-1.729	-45.184	114.085	1.00	21.40	A	C
35	ATOM	1125	C	LEU	242	-1.857	-47.667	116.161	1.00	20.42	A	C
	ATOM	1126	O	LEU	242	-2.585	-46.821	116.678	1.00	18.91	A	O
	ATOM	1127	N	PHE	243	-2.231	-48.929	115.981	1.00	20.27	A	N
	ATOM	1128	CA	PHE	243	-3.545	-49.390	116.386	1.00	20.87	A	C
	ATOM	1129	CB	PHE	243	-3.828	-50.766	115.775	1.00	21.22	A	C
40	ATOM	1130	CG	PHE	243	-4.211	-50.704	114.309	1.00	21.05	A	C
	ATOM	1131	CD1	PHE	243	-3.316	-50.212	113.359	1.00	19.68	A	C
	ATOM	1132	CD2	PHE	243	-5.478	-51.092	113.893	1.00	19.34	A	C
	ATOM	1133	CE1	PHE	243	-3.678	-50.104	112.022	1.00	20.59	A	C
	ATOM	1134	CE2	PHE	243	-5.850	-50.987	112.558	1.00	19.75	A	C
45	ATOM	1135	CZ	PHE	243	-4.950	-50.492	111.621	1.00	20.16	A	C
	ATOM	1136	C	PHE	243	-3.735	-49.402	117.899	1.00	21.36	A	C
	ATOM	1137	O	PHE	243	-4.855	-49.217	118.385	1.00	20.70	A	O
	ATOM	1138	N	HIS	244	-2.652	-49.608	118.644	1.00	21.51	A	N
	ATOM	1139	CA	HIS	244	-2.747	-49.586	120.101	1.00	22.59	A	C
50	ATOM	1140	CB	HIS	244	-1.448	-50.061	120.757	1.00	24.95	A	C
	ATOM	1141	CG	HIS	244	-1.424	-49.877	122.245	1.00	27.50	A	C
	ATOM	1142	CD2	HIS	244	-1.780	-50.711	123.252	1.00	28.29	A	C
	ATOM	1143	ND1	HIS	244	-1.033	-48.698	122.846	1.00	28.64	A	N
	ATOM	1144	CE1	HIS	244	-1.148	-48.814	124.157	1.00	29.14	A	C
55	ATOM	1145	NE2	HIS	244	-1.600	-50.025	124.430	1.00	29.46	A	N
	ATOM	1146	C	HIS	244	-3.029	-48.148	120.503	1.00	21.62	A	C
	ATOM	1147	O	HIS	244	-3.835	-47.897	121.394	1.00	21.60	A	O
	ATOM	1148	N	PHE	245	-2.355	-47.211	119.844	1.00	20.43	A	N
	ATOM	1149	CA	PHE	245	-2.560	-45.793	120.106	1.00	20.28	A	C
55	ATOM	1150	CB	PHE	245	-1.700	-44.935	119.173	1.00	19.48	A	C
	ATOM	1151	CG	PHE	245	-2.127	-43.495	119.121	1.00	20.46	A	C
	ATOM	1152	CD1	PHE	245	-1.755	-42.606	120.122	1.00	20.84	A	C

-189-

5	ATOM	1153	CD2	PHE	245	-2.957	-43.041	118.102	1.00	20.72	A	C
	ATOM	1154	CE1	PHE	245	-2.206	-41.284	120.113	1.00	19.78	A	C
	ATOM	1155	CE2	PHE	245	-3.413	-41.721	118.084	1.00	21.00	A	C
	ATOM	1156	CZ	PHE	245	-3.034	-40.844	119.096	1.00	20.53	A	C
	ATOM	1157	C	PHE	245	-4.033	-45.446	119.873	1.00	19.25	A	C
10	ATOM	1158	O	PHE	245	-4.676	-44.833	120.721	1.00	19.06	A	O
	ATOM	1159	N	HIS	246	-4.564	-45.844	118.722	1.00	19.01	A	N
	ATOM	1160	CA	HIS	246	-5.954	-45.546	118.400	1.00	19.09	A	C
	ATOM	1161	CB	HIS	246	-6.268	-45.962	116.953	1.00	18.50	A	C
	ATOM	1162	CG	HIS	246	-5.954	-44.898	115.944	1.00	18.48	A	C
15	ATOM	1163	CD2	HIS	246	-4.970	-44.805	115.018	1.00	18.21	A	C
	ATOM	1164	ND1	HIS	246	-6.665	-43.719	115.863	1.00	18.52	A	N
	ATOM	1165	CE1	HIS	246	-6.130	-42.945	114.935	1.00	17.66	A	C
	ATOM	1166	NE2	HIS	246	-5.100	-43.581	114.407	1.00	18.46	A	N
	ATOM	1167	C	HIS	246	-6.939	-46.185	119.377	1.00	18.38	A	C
20	ATOM	1168	O	HIS	246	-7.899	-45.550	119.801	1.00	18.13	A	O
	ATOM	1169	N	GLY	247	-6.704	-47.436	119.739	1.00	19.24	A	N
	ATOM	1170	CA	GLY	247	-7.596	-48.090	120.680	1.00	19.94	A	C
	ATOM	1171	C	GLY	247	-7.567	-47.385	122.022	1.00	20.61	A	C
	ATOM	1172	O	GLY	247	-8.615	-47.103	122.602	1.00	20.87	A	O
25	ATOM	1173	N	THR	248	-6.365	-47.084	122.511	1.00	19.95	A	N
	ATOM	1174	CA	THR	248	-6.211	-46.413	123.793	1.00	20.64	A	C
	ATOM	1175	CB	THR	248	-4.710	-46.204	124.144	1.00	21.09	A	C
	ATOM	1176	OG1	THR	248	-4.030	-47.467	124.116	1.00	21.47	A	O
	ATOM	1177	CG2	THR	248	-4.562	-45.601	125.534	1.00	18.96	A	C
30	ATOM	1178	C	THR	248	-6.922	-45.058	123.814	1.00	20.66	A	C
	ATOM	1179	O	THR	248	-7.642	-44.736	124.766	1.00	20.22	A	O
	ATOM	1180	N	LEU	249	-6.725	-44.270	122.761	1.00	21.23	A	N
	ATOM	1181	CA	LEU	249	-7.349	-42.953	122.674	1.00	21.39	A	C
	ATOM	1182	CB	LEU	249	-6.799	-42.178	121.471	1.00	21.91	A	C
35	ATOM	1183	CG	LEU	249	-7.341	-40.751	121.301	1.00	22.61	A	C
	ATOM	1184	CD1	LEU	249	-6.921	-39.910	122.494	1.00	23.51	A	C
	ATOM	1185	CD2	LEU	249	-6.818	-40.133	120.014	1.00	22.87	A	C
	ATOM	1186	C	LEU	249	-8.870	-43.036	122.569	1.00	20.82	A	C
	ATOM	1187	O	LEU	249	-9.573	-42.221	123.152	1.00	19.80	A	O
40	ATOM	1188	N	ARG	250	-9.374	-44.023	121.828	1.00	21.20	A	N
	ATOM	1189	CA	ARG	250	-10.816	-44.185	121.644	1.00	21.98	A	C
	ATOM	1190	CB	ARG	250	-11.100	-45.245	120.573	1.00	21.92	A	C
	ATOM	1191	CG	ARG	250	-12.563	-45.341	120.158	1.00	21.63	A	C
	ATOM	1192	CD	ARG	250	-12.994	-44.086	119.412	1.00	24.25	A	C
45	ATOM	1193	NE	ARG	250	-13.967	-44.395	118.368	1.00	25.98	A	N
	ATOM	1194	CZ	ARG	250	-15.285	-44.293	118.503	1.00	27.08	A	C
	ATOM	1195	NH1	ARG	250	-15.813	-43.874	119.644	1.00	27.73	A	N
	ATOM	1196	NH2	ARG	250	-16.077	-44.637	117.495	1.00	27.60	A	N
	ATOM	1197	C	ARG	250	-11.532	-44.580	122.936	1.00	22.80	A	C
50	ATOM	1198	O	ARG	250	-12.645	-44.126	123.194	1.00	22.12	A	O
	ATOM	1199	N	LYS	251	-10.893	-45.431	123.735	1.00	23.54	A	N
	ATOM	1200	CA	LYS	251	-11.471	-45.890	124.997	1.00	24.94	A	C
	ATOM	1201	CB	LYS	251	-10.576	-46.944	125.650	1.00	25.92	A	C
	ATOM	1202	CG	LYS	251	-10.575	-48.298	124.961	1.00	29.26	A	C
55	ATOM	1203	CD	LYS	251	-9.656	-49.271	125.690	1.00	30.89	A	C
	ATOM	1204	CE	LYS	251	-9.448	-50.550	124.889	1.00	33.42	A	C
	ATOM	1205	NZ	LYS	251	-8.346	-51.387	125.462	1.00	35.04	A	N
	ATOM	1206	C	LYS	251	-11.690	-44.754	125.992	1.00	25.07	A	C
	ATOM	1207	O	LYS	251	-12.468	-44.891	126.932	1.00	25.41	A	O
	ATOM	1208	N	LEU	252	-10.996	-43.639	125.793	1.00	24.90	A	N
	ATOM	1209	CA	LEU	252	-11.138	-42.499	126.685	1.00	25.36	A	C
	ATOM	1210	CB	LEU	252	-9.953	-41.549	126.503	1.00	23.70	A	C

-190-

	ATOM	1211	CG	LEU	252	-8.638	-42.172	126.985	1.00	24.00	A	C
	ATOM	1212	CD1	LEU	252	-7.491	-41.176	126.828	1.00	22.17	A	C
	ATOM	1213	CD2	LEU	252	-8.794	-42.599	128.449	1.00	21.31	A	C
5	ATOM	1214	C	LEU	252	-12.457	-41.748	126.504	1.00	26.07	A	C
	ATOM	1215	O	LEU	252	-12.822	-40.928	127.343	1.00	25.67	A	O
	ATOM	1216	N	GLN	253	-13.165	-42.027	125.410	1.00	27.09	A	N
	ATOM	1217	CA	GLN	253	-14.454	-41.394	125.142	1.00	28.60	A	C
	ATOM	1218	CB	GLN	253	-15.498	-41.944	126.122	1.00	30.52	A	C
10	ATOM	1219	CG	GLN	253	-15.871	-43.417	125.905	1.00	34.58	A	C
	ATOM	1220	CD	GLN	253	-16.676	-44.004	127.072	1.00	37.32	A	C
	ATOM	1221	OE1	GLN	253	-17.588	-43.365	127.602	1.00	38.93	A	O
	ATOM	1222	NE2	GLN	253	-16.341	-45.228	127.466	1.00	38.76	A	N
	ATOM	1223	C	GLN	253	-14.396	-39.866	125.246	1.00	28.46	A	C
15	ATOM	1224	O	GLN	253	-15.168	-39.256	125.986	1.00	28.32	A	O
	ATOM	1225	N	LEU	254	-13.487	-39.254	124.494	1.00	27.65	A	N
	ATOM	1226	CA	LEU	254	-13.323	-37.806	124.510	1.00	27.11	A	C
	ATOM	1227	CB	LEU	254	-12.011	-37.410	123.821	1.00	25.42	A	C
	ATOM	1228	CG	LEU	254	-10.698	-37.954	124.384	1.00	24.68	A	C
20	ATOM	1229	CD1	LEU	254	-9.530	-37.337	123.621	1.00	23.56	A	C
	ATOM	1230	CD2	LEU	254	-10.599	-37.627	125.867	1.00	23.28	A	C
	ATOM	1231	C	LEU	254	-14.467	-37.078	123.817	1.00	27.57	A	C
	ATOM	1232	O	LEU	254	-15.163	-37.642	122.974	1.00	26.67	A	O
	ATOM	1233	N	GLN	255	-14.648	-35.814	124.176	1.00	28.10	A	N
25	ATOM	1234	CA	GLN	255	-15.676	-34.990	123.562	1.00	29.49	A	C
	ATOM	1235	CB	GLN	255	-16.329	-34.095	124.616	1.00	31.52	A	C
	ATOM	1236	CG	GLN	255	-16.861	-34.865	125.810	1.00	35.22	A	C
	ATOM	1237	CD	GLN	255	-17.594	-33.978	126.791	1.00	38.55	A	C
	ATOM	1238	OE1	GLN	255	-17.099	-32.918	127.185	1.00	39.64	A	O
30	ATOM	1239	NE2	GLN	255	-18.784	-34.410	127.199	1.00	40.55	A	N
	ATOM	1240	C	GLN	255	-14.978	-34.145	122.496	1.00	28.88	A	C
	ATOM	1241	O	GLN	255	-13.778	-33.896	122.594	1.00	28.44	A	O
	ATOM	1242	N	GLU	256	-15.718	-33.718	121.478	1.00	28.49	A	N
	ATOM	1243	CA	GLU	256	-15.144	-32.912	120.405	1.00	28.54	A	C
35	ATOM	1244	CB	GLU	256	-16.240	-32.201	119.607	1.00	30.20	A	C
	ATOM	1245	CG	GLU	256	-16.750	-32.974	118.410	1.00	33.85	A	C
	ATOM	1246	CD	GLU	256	-17.234	-32.053	117.304	1.00	35.60	A	C
	ATOM	1247	OE1	GLU	256	-18.123	-31.214	117.567	1.00	37.88	A	O
	ATOM	1248	OE2	GLU	256	-16.723	-32.164	116.174	1.00	35.27	A	O
40	ATOM	1249	C	GLU	256	-14.118	-31.873	120.848	1.00	27.93	A	C
	ATOM	1250	O	GLU	256	-13.018	-31.823	120.319	1.00	27.24	A	O
	ATOM	1251	N	PRO	257	-14.471	-31.013	121.813	1.00	28.04	A	N
	ATOM	1252	CD	PRO	257	-15.754	-30.862	122.517	1.00	28.01	A	C
	ATOM	1253	CA	PRO	257	-13.502	-30.002	122.254	1.00	27.60	A	C
45	ATOM	1254	CB	PRO	257	-14.247	-29.261	123.371	1.00	28.41	A	C
	ATOM	1255	CG	PRO	257	-15.324	-30.241	123.795	1.00	29.41	A	C
	ATOM	1256	C	PRO	257	-12.150	-30.561	122.698	1.00	26.72	A	C
	ATOM	1257	O	PRO	257	-11.111	-29.957	122.436	1.00	27.19	A	O
	ATOM	1258	N	GLU	258	-12.163	-31.713	123.357	1.00	25.36	A	N
50	ATOM	1259	CA	GLU	258	-10.928	-32.343	123.818	1.00	24.44	A	C
	ATOM	1260	CB	GLU	258	-11.253	-33.457	124.813	1.00	24.01	A	C
	ATOM	1261	CG	GLU	258	-12.034	-32.924	126.004	1.00	26.10	A	C
	ATOM	1262	CD	GLU	258	-12.570	-34.006	126.911	1.00	26.63	A	C
	ATOM	1263	OE1	GLU	258	-13.128	-34.998	126.397	1.00	26.48	A	O
55	ATOM	1264	OE2	GLU	258	-12.446	-33.853	128.143	1.00	28.74	A	O
	ATOM	1265	C	GLU	258	-10.116	-32.876	122.637	1.00	23.76	A	C
	ATOM	1266	O	GLU	258	-8.893	-32.779	122.634	1.00	22.67	A	O
	ATOM	1267	N	TYR	259	-10.796	-33.427	121.634	1.00	22.12	A	N
	ATOM	1268	CA	TYR	259	-10.108	-33.924	120.446	1.00	22.11	A	C

-191-

	ATOM	1269	CB	TYR	259	-11.091	-34.596	119.485	1.00	21.08	A	C
	ATOM	1270	CG	TYR	259	-11.261	-36.087	119.674	1.00	21.43	A	C
	ATOM	1271	CD1	TYR	259	-10.198	-36.970	119.442	1.00	21.24	A	C
5	ATOM	1272	CE1	TYR	259	-10.365	-38.354	119.561	1.00	19.51	A	C
	ATOM	1273	CD2	TYR	259	-12.493	-36.622	120.036	1.00	20.98	A	C
	ATOM	1274	CE2	TYR	259	-12.672	-38.003	120.157	1.00	21.07	A	C
	ATOM	1275	CZ	TYR	259	-11.601	-38.860	119.914	1.00	19.86	A	C
	ATOM	1276	OH	TYR	259	-11.788	-40.218	120.006	1.00	18.11	A	O
10	ATOM	1277	C	TYR	259	-9.466	-32.752	119.723	1.00	22.33	A	C
	ATOM	1278	O	TYR	259	-8.308	-32.817	119.295	1.00	21.92	A	O
	ATOM	1279	N	VAL	260	-10.229	-31.677	119.575	1.00	22.03	A	N
	ATOM	1280	CA	VAL	260	-9.727	-30.516	118.877	1.00	23.22	A	C
	ATOM	1281	CB	VAL	260	-10.856	-29.512	118.626	1.00	24.49	A	C
15	ATOM	1282	CG1	VAL	260	-10.293	-28.125	118.451	1.00	26.18	A	C
	ATOM	1283	CG2	VAL	260	-11.609	-29.913	117.372	1.00	24.67	A	C
	ATOM	1284	C	VAL	260	-8.557	-29.849	119.590	1.00	22.97	A	C
	ATOM	1285	O	VAL	260	-7.609	-29.416	118.937	1.00	22.35	A	O
	ATOM	1286	N	LEU	261	-8.620	-29.766	120.916	1.00	23.08	A	N
20	ATOM	1287	CA	LEU	261	-7.532	-29.161	121.679	1.00	24.42	A	C
	ATOM	1288	CB	LEU	261	-7.936	-28.975	123.145	1.00	24.90	A	C
	ATOM	1289	CG	LEU	261	-8.902	-27.817	123.411	1.00	24.74	A	C
	ATOM	1290	CD1	LEU	261	-9.489	-27.932	124.808	1.00	25.84	A	C
	ATOM	1291	CD2	LEU	261	-8.160	-26.501	123.235	1.00	24.89	A	C
25	ATOM	1292	C	LEU	261	-6.297	-30.053	121.576	1.00	24.56	A	C
	ATOM	1293	O	LEU	261	-5.170	-29.560	121.469	1.00	24.62	A	O
	ATOM	1294	N	LEU	262	-6.507	-31.367	121.602	1.00	24.08	A	N
	ATOM	1295	CA	LEU	262	-5.393	-32.300	121.473	1.00	24.35	A	C
	ATOM	1296	CB	LEU	262	-5.901	-33.739	121.558	1.00	25.52	A	C
30	ATOM	1297	CG	LEU	262	-4.940	-34.844	122.018	1.00	26.64	A	C
	ATOM	1298	CD1	LEU	262	-4.394	-34.531	123.404	1.00	26.40	A	C
	ATOM	1299	CD2	LEU	262	-5.693	-36.172	122.044	1.00	26.95	A	C
	ATOM	1300	C	LEU	262	-4.729	-32.037	120.112	1.00	23.84	A	C
	ATOM	1301	O	LEU	262	-3.504	-32.002	120.009	1.00	23.68	A	O
35	ATOM	1302	N	ALA	263	-5.535	-31.833	119.071	1.00	22.30	A	N
	ATOM	1303	CA	ALA	263	-4.987	-31.551	117.749	1.00	22.57	A	C
	ATOM	1304	CB	ALA	263	-6.102	-31.473	116.710	1.00	21.76	A	C
	ATOM	1305	C	ALA	263	-4.210	-30.234	117.779	1.00	22.78	A	C
	ATOM	1306	O	ALA	263	-3.136	-30.126	117.186	1.00	22.16	A	O
40	ATOM	1307	N	ALA	264	-4.762	-29.239	118.470	1.00	22.57	A	N
	ATOM	1308	CA	ALA	264	-4.123	-27.934	118.586	1.00	24.00	A	C
	ATOM	1309	CB	ALA	264	-5.043	-26.965	119.332	1.00	23.05	A	C
	ATOM	1310	C	ALA	264	-2.772	-28.043	119.302	1.00	24.41	A	C
	ATOM	1311	O	ALA	264	-1.814	-27.357	118.944	1.00	24.83	A	O
45	ATOM	1312	N	MET	265	-2.699	-28.904	120.312	1.00	25.02	A	N
	ATOM	1313	CA	MET	265	-1.462	-29.094	121.055	1.00	25.93	A	C
	ATOM	1314	CB	MET	265	-1.720	-29.938	122.306	1.00	26.79	A	C
	ATOM	1315	CG	MET	265	-2.440	-29.175	123.415	1.00	27.47	A	C
	ATOM	1316	SD	MET	265	-2.957	-30.218	124.797	1.00	28.87	A	S
50	ATOM	1317	CE	MET	265	-1.384	-30.422	125.669	1.00	27.94	A	C
	ATOM	1318	C	MET	265	-0.404	-29.751	120.177	1.00	26.28	A	C
	ATOM	1319	O	MET	265	0.785	-29.434	120.276	1.00	26.21	A	O
	ATOM	1320	N	ALA	266	-0.830	-30.667	119.314	1.00	25.89	A	N
	ATOM	1321	CA	ALA	266	0.112	-31.328	118.417	1.00	25.79	A	C
55	ATOM	1322	CB	ALA	266	-0.570	-32.488	117.700	1.00	24.34	A	C
	ATOM	1323	C	ALA	266	0.616	-30.295	117.402	1.00	26.44	A	C
	ATOM	1324	O	ALA	266	1.801	-30.272	117.060	1.00	25.58	A	O
	ATOM	1325	N	LEU	267	-0.292	-29.439	116.936	1.00	26.96	A	N
	ATOM	1326	CA	LEU	267	0.041	-28.401	115.968	1.00	29.21	A	C

-192-

	ATOM	1327	CB	LEU	267	-1.218	-27.636	115.547	1.00	28.28	A	C
	ATOM	1328	CG	LEU	267	-1.322	-27.086	114.116	1.00	28.22	A	C
	ATOM	1329	CD1	LEU	267	-2.153	-25.815	114.151	1.00	26.62	A	C
5	ATOM	1330	CD2	LEU	267	0.040	-26.797	113.520	1.00	27.55	A	C
	ATOM	1331	C	LEU	267	1.051	-27.405	116.541	1.00	30.31	A	C
	ATOM	1332	O	LEU	267	2.114	-27.195	115.966	1.00	30.73	A	O
	ATOM	1333	N	PHE	268	0.720	-26.795	117.674	1.00	31.98	A	N
	ATOM	1334	CA	PHE	268	1.615	-25.817	118.281	1.00	34.42	A	C
10	ATOM	1335	CB	PHE	268	0.811	-24.778	119.065	1.00	33.07	A	C
	ATOM	1336	CG	PHE	268	-0.129	-23.980	118.209	1.00	33.01	A	C
	ATOM	1337	CD1	PHE	268	-1.497	-24.236	118.224	1.00	31.94	A	C
	ATOM	1338	CD2	PHE	268	0.357	-22.995	117.356	1.00	32.71	A	C
	ATOM	1339	CE1	PHE	268	-2.366	-23.526	117.402	1.00	31.94	A	C
	ATOM	1340	CE2	PHE	268	-0.507	-22.278	116.527	1.00	32.75	A	C
15	ATOM	1341	CZ	PHE	268	-1.871	-22.545	116.551	1.00	32.01	A	C
	ATOM	1342	C	PHE	268	2.690	-26.424	119.171	1.00	35.98	A	C
	ATOM	1343	O	PHE	268	2.635	-26.328	120.393	1.00	36.42	A	O
	ATOM	1344	N	SER	269	3.672	-27.050	118.537	1.00	38.74	A	N
20	ATOM	1345	CA	SER	269	4.785	-27.669	119.244	1.00	41.31	A	C
	ATOM	1346	CB	SER	269	5.001	-29.096	118.743	1.00	41.54	A	C
	ATOM	1347	OG	SER	269	3.849	-29.890	118.970	1.00	43.06	A	O
	ATOM	1348	C	SER	269	6.026	-26.834	118.969	1.00	42.81	A	C
	ATOM	1349	O	SER	269	6.505	-26.782	117.840	1.00	43.23	A	O
	ATOM	1350	N	PRO	270	6.564	-26.171	120.002	1.00	44.83	A	N
25	ATOM	1351	CD	PRO	270	6.116	-26.232	121.406	1.00	44.95	A	C
	ATOM	1352	CA	PRO	270	7.758	-25.326	119.873	1.00	46.18	A	C
	ATOM	1353	CB	PRO	270	7.883	-24.699	121.259	1.00	45.92	A	C
	ATOM	1354	CG	PRO	270	7.351	-25.782	122.156	1.00	45.81	A	C
30	ATOM	1355	C	PRO	270	9.034	-26.055	119.452	1.00	47.67	A	C
	ATOM	1356	O	PRO	270	9.967	-25.437	118.935	1.00	48.27	A	O
	ATOM	1357	N	ASP	271	9.078	-27.365	119.672	1.00	48.67	A	N
	ATOM	1358	CA	ASP	271	10.256	-28.147	119.321	1.00	49.58	A	C
	ATOM	1359	CB	ASP	271	10.531	-29.191	120.409	1.00	50.08	A	C
35	ATOM	1360	CG	ASP	271	9.369	-30.141	120.621	1.00	50.89	A	C
	ATOM	1361	OD1	ASP	271	8.217	-29.676	120.767	1.00	51.46	A	O
	ATOM	1362	OD2	ASP	271	9.611	-31.362	120.658	1.00	51.73	A	O
	ATOM	1363	C	ASP	271	10.168	-28.815	117.950	1.00	50.08	A	C
	ATOM	1364	O	ASP	271	10.933	-29.731	117.644	1.00	50.01	A	O
40	ATOM	1365	N	ARG	272	9.238	-28.351	117.124	1.00	50.50	A	N
	ATOM	1366	CA	ARG	272	9.082	-28.895	115.784	1.00	51.11	A	C
	ATOM	1367	CB	ARG	272	7.824	-28.330	115.126	1.00	50.35	A	C
	ATOM	1368	CG	ARG	272	7.023	-29.341	114.325	1.00	49.50	A	C
	ATOM	1369	CD	ARG	272	5.919	-29.977	115.161	1.00	48.07	A	C
45	ATOM	1370	NE	ARG	272	6.151	-31.394	115.405	1.00	47.04	A	N
	ATOM	1371	CZ	ARG	272	5.237	-32.240	115.873	1.00	45.93	A	C
	ATOM	1372	NH1	ARG	272	4.011	-31.822	116.154	1.00	45.21	A	N
	ATOM	1373	NH2	ARG	272	5.553	-33.512	116.062	1.00	44.85	A	N
	ATOM	1374	C	ARG	272	10.317	-28.449	115.005	1.00	51.77	A	C
50	ATOM	1375	O	ARG	272	10.674	-27.271	115.015	1.00	52.46	A	O
	ATOM	1376	N	PRO	273	10.987	-29.380	114.317	1.00	52.32	A	N
	ATOM	1377	CD	PRO	273	10.581	-30.768	114.035	1.00	52.48	A	C
	ATOM	1378	CA	PRO	273	12.186	-29.020	113.552	1.00	52.55	A	C
	ATOM	1379	CB	PRO	273	12.567	-30.337	112.876	1.00	52.49	A	C
55	ATOM	1380	CG	PRO	273	11.241	-31.023	112.706	1.00	52.55	A	C
	ATOM	1381	C	PRO	273	11.998	-27.879	112.550	1.00	52.78	A	C
	ATOM	1382	O	PRO	273	11.186	-27.978	111.628	1.00	52.86	A	O
	ATOM	1383	N	GLY	274	12.747	-26.796	112.742	1.00	52.71	A	N
	ATOM	1384	CA	GLY	274	12.661	-25.668	111.831	1.00	52.86	A	C

-193-

	ATOM	1385	C	GLY	274	11.921	-24.428	112.306	1.00	53.31	A	C
	ATOM	1386	O	GLY	274	11.825	-23.448	111.567	1.00	52.74	A	O
	ATOM	1387	N	VAL	275	11.396	-24.451	113.526	1.00	53.86	A	N
	ATOM	1388	CA	VAL	275	10.668	-23.294	114.041	1.00	54.72	A	C
5	ATOM	1389	CB	VAL	275	9.849	-23.653	115.302	1.00	54.41	A	C
	ATOM	1390	CG1	VAL	275	8.906	-24.806	114.998	1.00	54.40	A	C
	ATOM	1391	CG2	VAL	275	10.781	-24.010	116.448	1.00	54.73	A	C
	ATOM	1392	C	VAL	275	11.620	-22.152	114.391	1.00	55.42	A	C
10	ATOM	1393	O	VAL	275	12.793	-22.376	114.694	1.00	55.34	A	O
	ATOM	1394	N	THR	276	11.103	-20.928	114.341	1.00	56.25	A	N
	ATOM	1395	CA	THR	276	11.888	-19.738	114.657	1.00	57.04	A	C
	ATOM	1396	CB	THR	276	12.019	-18.806	113.428	1.00	57.12	A	C
	ATOM	1397	OG1	THR	276	10.728	-18.310	113.054	1.00	57.58	A	O
	ATOM	1398	CG2	THR	276	12.624	-19.559	112.252	1.00	56.94	A	C
15	ATOM	1399	C	THR	276	11.249	-18.958	115.810	1.00	57.44	A	C
	ATOM	1400	O	THR	276	11.939	-18.283	116.573	1.00	57.90	A	O
	ATOM	1401	N	GLN	277	9.928	-19.058	115.929	1.00	57.58	A	N
	ATOM	1402	CA	GLN	277	9.183	-18.383	116.987	1.00	57.56	A	C
20	ATOM	1403	CB	GLN	277	7.827	-17.912	116.453	1.00	57.96	A	C
	ATOM	1404	CG	GLN	277	7.476	-16.472	116.777	1.00	59.08	A	C
	ATOM	1405	CD	GLN	277	7.893	-15.506	115.683	1.00	59.41	A	C
	ATOM	1406	OE1	GLN	277	9.063	-15.444	115.303	1.00	60.10	A	O
	ATOM	1407	NE2	GLN	277	6.933	-14.746	115.171	1.00	59.47	A	N
25	ATOM	1408	C	GLN	277	8.953	-19.379	118.125	1.00	57.42	A	C
	ATOM	1409	O	GLN	277	7.836	-19.507	118.629	1.00	57.26	A	O
	ATOM	1410	N	ARG	278	10.009	-20.078	118.531	1.00	57.27	A	N
	ATOM	1411	CA	ARG	278	9.899	-21.080	119.585	1.00	57.49	A	C
	ATOM	1412	CB	ARG	278	11.279	-21.630	119.951	1.00	58.82	A	C
30	ATOM	1413	CG	ARG	278	11.208	-22.952	120.705	1.00	60.52	A	C
	ATOM	1414	CD	ARG	278	12.581	-23.453	121.124	1.00	62.18	A	C
	ATOM	1415	NE	ARG	278	12.567	-24.877	121.465	1.00	63.94	A	N
	ATOM	1416	CZ	ARG	278	11.915	-25.415	122.495	1.00	64.51	A	C
	ATOM	1417	NH1	ARG	278	11.979	-26.725	122.697	1.00	64.55	A	N
35	ATOM	1418	NH2	ARG	278	11.209	-24.656	123.328	1.00	64.96	A	N
	ATOM	1419	C	ARG	278	9.198	-20.593	120.851	1.00	56.92	A	C
	ATOM	1420	O	ARG	278	8.325	-21.281	121.380	1.00	56.95	A	O
	ATOM	1421	N	ASP	279	9.578	-19.419	121.344	1.00	56.06	A	N
	ATOM	1422	CA	ASP	279	8.956	-18.883	122.551	1.00	55.37	A	C
40	ATOM	1423	CB	ASP	279	9.646	-17.588	122.990	1.00	56.68	A	C
	ATOM	1424	CG	ASP	279	11.084	-17.809	123.419	1.00	57.63	A	C
	ATOM	1425	OD1	ASP	279	11.930	-18.105	122.547	1.00	58.84	A	O
	ATOM	1426	OD2	ASP	279	11.367	-17.692	124.629	1.00	58.07	A	O
	ATOM	1427	C	ASP	279	7.470	-18.618	122.338	1.00	54.14	A	C
45	ATOM	1428	O	ASP	279	6.639	-19.007	123.156	1.00	53.64	A	O
	ATOM	1429	N	GLU	280	7.142	-17.955	121.235	1.00	52.98	A	N
	ATOM	1430	CA	GLU	280	5.759	-17.634	120.918	1.00	51.96	A	C
	ATOM	1431	CB	GLU	280	5.691	-16.869	119.598	1.00	52.88	A	C
	ATOM	1432	CG	GLU	280	4.345	-16.227	119.329	1.00	54.43	A	C
50	ATOM	1433	CD	GLU	280	4.264	-15.603	117.951	1.00	55.52	A	C
	ATOM	1434	OE1	GLU	280	5.204	-14.875	117.570	1.00	56.15	A	O
	ATOM	1435	OE2	GLU	280	3.255	-15.834	117.252	1.00	55.94	A	O
	ATOM	1436	C	GLU	280	4.908	-18.898	120.821	1.00	50.62	A	C
	ATOM	1437	O	GLU	280	3.869	-19.007	121.470	1.00	50.58	A	O
55	ATOM	1438	N	ILE	281	5.357	-19.847	120.004	1.00	49.04	A	N
	ATOM	1439	CA	ILE	281	4.649	-21.113	119.815	1.00	47.41	A	C
	ATOM	1440	CB	ILE	281	5.366	-21.997	118.764	1.00	46.53	A	C
	ATOM	1441	CG2	ILE	281	4.672	-23.349	118.655	1.00	45.22	A	C
	ATOM	1442	CG1	ILE	281	5.378	-21.282	117.408	1.00	45.56	A	C

-194-

	ATOM	1443	CD1	ILE	281	6.138	-22.010	116.326	1.00	45.01	A	C
	ATOM	1444	C	ILE	281	4.533	-21.886	121.131	1.00	47.29	A	C
	ATOM	1445	O	ILE	281	3.525	-22.549	121.383	1.00	46.81	A	O
5	ATOM	1446	N	ASP	282	5.568	-21.797	121.965	1.00	46.94	A	N
	ATOM	1447	CA	ASP	282	5.574	-22.471	123.260	1.00	46.55	A	C
	ATOM	1448	CB	ASP	282	6.946	-22.311	123.926	1.00	47.68	A	C
	ATOM	1449	CG	ASP	282	7.098	-23.166	125.170	1.00	48.85	A	C
	ATOM	1450	OD1	ASP	282	6.921	-24.402	125.082	1.00	49.57	A	O
10	ATOM	1451	OD2	ASP	282	7.402	-22.602	126.242	1.00	49.92	A	O
	ATOM	1452	C	ASP	282	4.470	-21.876	124.144	1.00	45.75	A	C
	ATOM	1453	O	ASP	282	3.847	-22.583	124.934	1.00	45.36	A	O
	ATOM	1454	N	GLN	283	4.226	-20.576	124.000	1.00	45.11	A	N
	ATOM	1455	CA	GLN	283	3.181	-19.904	124.770	1.00	45.13	A	C
15	ATOM	1456	CB	GLN	283	3.256	-18.387	124.563	1.00	46.75	A	C
	ATOM	1457	CG	GLN	283	2.563	-17.534	125.637	1.00	50.09	A	C
	ATOM	1458	CD	GLN	283	1.092	-17.879	125.849	1.00	52.42	A	C
	ATOM	1459	OE1	GLN	283	0.754	-18.757	126.649	1.00	54.11	A	O
	ATOM	1460	NE2	GLN	283	0.210	-17.189	125.129	1.00	53.63	A	N
20	ATOM	1461	C	GLN	283	1.821	-20.423	124.292	1.00	43.58	A	C
	ATOM	1462	O	GLN	283	0.929	-20.680	125.099	1.00	43.49	A	O
	ATOM	1463	N	LEU	284	1.664	-20.573	122.979	1.00	42.02	A	N
	ATOM	1464	CA	LEU	284	0.409	-21.079	122.428	1.00	40.90	A	C
	ATOM	1465	CB	LEU	284	0.438	-21.086	120.892	1.00	40.60	A	C
25	ATOM	1466	CG	LEU	284	0.221	-19.783	120.110	1.00	40.12	A	C
	ATOM	1467	CD1	LEU	284	-0.648	-18.833	120.918	1.00	39.50	A	C
	ATOM	1468	CD2	LEU	284	1.551	-19.146	119.789	1.00	40.64	A	C
	ATOM	1469	C	LEU	284	0.140	-22.491	122.934	1.00	39.59	A	C
	ATOM	1470	O	LEU	284	-0.986	-22.825	123.292	1.00	39.24	A	O
30	ATOM	1471	N	GLN	285	1.180	-23.318	122.950	1.00	39.22	A	N
	ATOM	1472	CA	GLN	285	1.070	-24.688	123.433	1.00	38.77	A	C
	ATOM	1473	CB	GLN	285	2.454	-25.344	123.452	1.00	39.75	A	C
	ATOM	1474	CG	GLN	285	2.497	-26.740	124.049	1.00	42.43	A	C
	ATOM	1475	CD	GLN	285	1.934	-27.788	123.117	1.00	43.45	A	C
35	ATOM	1476	OE1	GLN	285	0.771	-27.728	122.730	1.00	45.03	A	O
	ATOM	1477	NE2	GLN	285	2.763	-28.757	122.747	1.00	44.86	A	N
	ATOM	1478	C	GLN	285	0.487	-24.653	124.843	1.00	37.86	A	C
	ATOM	1479	O	GLN	285	-0.501	-25.323	125.138	1.00	37.02	A	O
	ATOM	1480	N	GLU	286	1.096	-23.851	125.710	1.00	37.54	A	N
40	ATOM	1481	CA	GLU	286	0.628	-23.736	127.085	1.00	37.97	A	C
	ATOM	1482	CB	GLU	286	1.526	-22.794	127.884	1.00	39.37	A	C
	ATOM	1483	CG	GLU	286	2.269	-23.502	128.993	1.00	42.37	A	C
	ATOM	1484	CD	GLU	286	1.361	-24.415	129.792	1.00	44.10	A	C
	ATOM	1485	OE1	GLU	286	0.394	-23.910	130.402	1.00	45.20	A	O
45	ATOM	1486	OE2	GLU	286	1.612	-25.640	129.803	1.00	46.83	A	O
	ATOM	1487	C	GLU	286	-0.808	-23.257	127.167	1.00	36.84	A	C
	ATOM	1488	O	GLU	286	-1.552	-23.668	128.047	1.00	36.65	A	O
	ATOM	1489	N	GLU	287	-1.187	-22.376	126.251	1.00	37.13	A	N
	ATOM	1490	CA	GLU	287	-2.541	-21.848	126.203	1.00	37.20	A	C
50	ATOM	1491	CB	GLU	287	-2.625	-20.761	125.128	1.00	39.14	A	C
	ATOM	1492	CG	GLU	287	-3.881	-19.906	125.181	1.00	42.57	A	C
	ATOM	1493	CD	GLU	287	-3.893	-18.822	124.108	1.00	44.54	A	C
	ATOM	1494	OE1	GLU	287	-2.923	-18.031	124.049	1.00	45.67	A	O
	ATOM	1495	OE2	GLU	287	-4.873	-18.762	123.330	1.00	45.07	A	O
55	ATOM	1496	C	GLU	287	-3.517	-22.987	125.885	1.00	36.19	A	C
	ATOM	1497	O	GLU	287	-4.565	-23.109	126.514	1.00	35.33	A	O
	ATOM	1498	N	MET	288	-3.161	-23.819	124.907	1.00	35.38	A	N
	ATOM	1499	CA	MET	288	-3.998	-24.950	124.509	1.00	34.70	A	C
	ATOM	1500	CB	MET	288	-3.384	-25.689	123.313	1.00	35.45	A	C

-195-

	ATOM	1501	CG	MET	288	-3.064	-24.841	122.100	1.00	36.49	A	C
	ATOM	1502	SD	MET	288	-4.518	-24.110	121.347	1.00	37.77	A	S
	ATOM	1503	CE	MET	288	-4.196	-22.370	121.637	1.00	38.91	A	C
5	ATOM	1504	C	MET	288	-4.108	-25.930	125.671	1.00	33.74	A	C
	ATOM	1505	O	MET	288	-5.202	-26.379	126.025	1.00	33.02	A	O
	ATOM	1506	N	ALA	289	-2.956	-26.260	126.253	1.00	33.19	A	N
	ATOM	1507	CA	ALA	289	-2.880	-27.195	127.370	1.00	32.47	A	C
	ATOM	1508	CB	ALA	289	-1.431	-27.340	127.826	1.00	31.87	A	C
10	ATOM	1509	C	ALA	289	-3.760	-26.772	128.541	1.00	32.22	A	C
	ATOM	1510	O	ALA	289	-4.537	-27.575	129.066	1.00	31.24	A	O
	ATOM	1511	N	LEU	290	-3.634	-25.512	128.948	1.00	32.24	A	N
	ATOM	1512	CA	LEU	290	-4.420	-24.985	130.055	1.00	32.90	A	C
	ATOM	1513	CB	LEU	290	-4.009	-23.543	130.348	1.00	34.69	A	C
15	ATOM	1514	CG	LEU	290	-2.627	-23.383	130.975	1.00	35.82	A	C
	ATOM	1515	CD1	LEU	290	-2.309	-21.900	131.153	1.00	36.30	A	C
	ATOM	1516	CD2	LEU	290	-2.601	-24.111	132.314	1.00	36.19	A	C
	ATOM	1517	C	LEU	290	-5.910	-25.050	129.761	1.00	32.17	A	C
	ATOM	1518	O	LEU	290	-6.707	-25.393	130.628	1.00	32.35	A	O
20	ATOM	1519	N	THR	291	-6.283	-24.713	128.533	1.00	31.75	A	N
	ATOM	1520	CA	THR	291	-7.680	-24.761	128.124	1.00	31.71	A	C
	ATOM	1521	CB	THR	291	-7.837	-24.298	126.662	1.00	32.01	A	C
	ATOM	1522	OG1	THR	291	-7.204	-23.022	126.497	1.00	32.68	A	O
	ATOM	1523	CG2	THR	291	-9.312	-24.179	126.291	1.00	31.69	A	C
25	ATOM	1524	C	THR	291	-8.192	-26.199	128.252	1.00	31.72	A	C
	ATOM	1525	O	THR	291	-9.289	-26.434	128.760	1.00	31.36	A	O
	ATOM	1526	N	LEU	292	-7.392	-27.159	127.792	1.00	31.96	A	N
	ATOM	1527	CA	LEU	292	-7.772	-28.567	127.864	1.00	32.82	A	C
	ATOM	1528	CB	LEU	292	-6.672	-29.464	127.278	1.00	31.84	A	C
30	ATOM	1529	CG	LEU	292	-7.088	-30.797	126.636	1.00	32.12	A	C
	ATOM	1530	CD1	LEU	292	-5.901	-31.753	126.649	1.00	30.55	A	C
	ATOM	1531	CD2	LEU	292	-8.265	-31.413	127.367	1.00	31.13	A	C
	ATOM	1532	C	LEU	292	-8.005	-28.960	129.318	1.00	33.29	A	C
	ATOM	1533	O	LEU	292	-9.011	-29.582	129.643	1.00	32.92	A	O
35	ATOM	1534	N	GLN	293	-7.061	-28.606	130.185	1.00	34.69	A	N
	ATOM	1535	CA	GLN	293	-7.170	-28.920	131.603	1.00	36.33	A	C
	ATOM	1536	CB	GLN	293	-5.973	-28.369	132.368	1.00	37.25	A	C
	ATOM	1537	CG	GLN	293	-4.664	-29.038	132.047	1.00	38.64	A	C
	ATOM	1538	CD	GLN	293	-3.551	-28.560	132.948	1.00	39.42	A	C
40	ATOM	1539	OE1	GLN	293	-3.615	-28.720	134.169	1.00	40.32	A	O
	ATOM	1540	NE2	GLN	293	-2.521	-27.966	132.355	1.00	39.89	A	N
	ATOM	1541	C	GLN	293	-8.444	-28.337	132.194	1.00	37.50	A	C
	ATOM	1542	O	GLN	293	-9.207	-29.043	132.852	1.00	37.40	A	O
	ATOM	1543	N	SER	294	-8.661	-27.044	131.969	1.00	38.47	A	N
45	ATOM	1544	CA	SER	294	-9.850	-26.367	132.480	1.00	39.65	A	C
	ATOM	1545	CB	SER	294	-9.890	-24.916	131.994	1.00	39.69	A	C
	ATOM	1546	OG	SER	294	-8.707	-24.222	132.355	1.00	40.48	A	O
	ATOM	1547	C	SER	294	-11.092	-27.098	131.996	1.00	40.07	A	C
	ATOM	1548	O	SER	294	-12.013	-27.358	132.770	1.00	40.28	A	O
50	ATOM	1549	N	TYR	295	-11.106	-27.439	130.712	1.00	40.29	A	N
	ATOM	1550	CA	TYR	295	-12.239	-28.135	130.129	1.00	41.02	A	C
	ATOM	1551	CB	TYR	295	-12.006	-28.362	128.633	1.00	40.48	A	C
	ATOM	1552	CG	TYR	295	-13.219	-28.921	127.941	1.00	40.03	A	C
	ATOM	1553	CD1	TYR	295	-13.535	-30.275	128.033	1.00	39.72	A	C
55	ATOM	1554	CE1	TYR	295	-14.708	-30.775	127.483	1.00	40.15	A	C
	ATOM	1555	CD2	TYR	295	-14.106	-28.080	127.271	1.00	39.70	A	C
	ATOM	1556	CE2	TYR	295	-15.279	-28.568	126.722	1.00	39.35	A	C
	ATOM	1557	CZ	TYR	295	-15.574	-29.915	126.834	1.00	40.12	A	C
	ATOM	1558	OH	TYR	295	-16.748	-30.399	126.308	1.00	41.32	A	O

-196-

5	ATOM	1559	C	TYR	295	-12.507	-29.465	130.824	1.00	41.79	A	C
	ATOM	1560	O	TYR	295	-13.649	-29.785	131.146	1.00	42.03	A	O
	ATOM	1561	N	ILE	296	-11.455	-30.241	131.051	1.00	42.99	A	N
	ATOM	1562	CA	ILE	296	-11.591	-31.532	131.711	1.00	44.15	A	C
	ATOM	1563	CB	ILE	296	-10.250	-32.290	131.718	1.00	43.14	A	C
	ATOM	1564	CG2	ILE	296	-10.377	-33.564	132.540	1.00	42.45	A	C
	ATOM	1565	CG1	ILE	296	-9.823	-32.597	130.279	1.00	42.93	A	C
10	ATOM	1566	CD1	ILE	296	-8.468	-33.258	130.163	1.00	41.86	A	C
	ATOM	1567	C	ILE	296	-12.080	-31.365	133.150	1.00	45.76	A	C
	ATOM	1568	O	ILE	296	-12.958	-32.099	133.604	1.00	45.29	A	O
	ATOM	1569	N	LYS	297	-11.508	-30.401	133.866	1.00	48.10	A	N
	ATOM	1570	CA	LYS	297	-11.901	-30.141	135.248	1.00	51.07	A	C
	ATOM	1571	CB	LYS	297	-11.079	-28.985	135.828	1.00	51.11	A	C
	ATOM	1572	CG	LYS	297	-9.628	-29.359	136.112	1.00	52.35	A	C
15	ATOM	1573	CD	LYS	297	-8.831	-28.200	136.696	1.00	53.18	A	C
	ATOM	1574	CE	LYS	297	-7.404	-28.635	137.020	1.00	54.08	A	C
	ATOM	1575	NZ	LYS	297	-6.565	-27.527	137.567	1.00	54.48	A	N
	ATOM	1576	C	LYS	297	-13.392	-29.835	135.362	1.00	53.02	A	C
	ATOM	1577	O	LYS	297	-14.038	-30.238	136.328	1.00	53.38	A	O
	ATOM	1578	N	GLY	298	-13.938	-29.132	134.374	1.00	55.42	A	N
	ATOM	1579	CA	GLY	298	-15.353	-28.810	134.397	1.00	58.64	A	C
20	ATOM	1580	C	GLY	298	-16.214	-29.936	133.854	1.00	61.18	A	C
	ATOM	1581	O	GLY	298	-17.337	-29.704	133.409	1.00	61.26	A	O
	ATOM	1582	N	GLN	299	-15.684	-31.156	133.895	1.00	63.92	A	N
	ATOM	1583	CA	GLN	299	-16.379	-32.344	133.405	1.00	66.98	A	C
	ATOM	1584	CB	GLN	299	-15.633	-33.613	133.853	1.00	67.13	A	C
	ATOM	1585	CG	GLN	299	-15.230	-33.657	135.333	1.00	67.29	A	C
	ATOM	1586	CD	GLN	299	-16.415	-33.750	136.282	1.00	67.70	A	C
30	ATOM	1587	OE1	GLN	299	-17.196	-34.701	136.230	1.00	67.82	A	O
	ATOM	1588	NE2	GLN	299	-16.551	-32.760	137.161	1.00	67.75	A	N
	ATOM	1589	C	GLN	299	-17.835	-32.416	133.850	1.00	68.93	A	C
	ATOM	1590	O	GLN	299	-18.228	-31.783	134.831	1.00	69.45	A	O
	ATOM	1591	N	GLN	300	-18.634	-33.186	133.116	1.00	71.11	A	N
	ATOM	1592	CA	GLN	300	-20.045	-33.340	133.446	1.00	73.14	A	C
	ATOM	1593	CB	GLN	300	-20.819	-33.903	132.250	1.00	73.51	A	C
35	ATOM	1594	CG	GLN	300	-21.287	-32.844	131.267	1.00	74.36	A	C
	ATOM	1595	CD	GLN	300	-22.243	-31.847	131.902	1.00	75.03	A	C
	ATOM	1596	OE1	GLN	300	-21.883	-31.131	132.842	1.00	75.24	A	O
	ATOM	1597	NE2	GLN	300	-23.471	-31.797	131.392	1.00	75.25	A	N
	ATOM	1598	C	GLN	300	-20.246	-34.235	134.661	1.00	74.34	A	C
	ATOM	1599	O	GLN	300	-20.722	-33.777	135.700	1.00	74.59	A	O
	ATOM	1600	N	ARG	301	-19.883	-35.509	134.543	1.00	75.65	A	N
45	ATOM	1601	CA	ARG	301	-20.049	-36.419	135.667	1.00	76.68	A	C
	ATOM	1602	CB	ARG	301	-21.478	-36.985	135.677	1.00	77.20	A	C
	ATOM	1603	CG	ARG	301	-21.959	-37.404	137.063	1.00	78.13	A	C
	ATOM	1604	CD	ARG	301	-23.132	-38.365	137.011	1.00	78.94	A	C
	ATOM	1605	NE	ARG	301	-23.446	-38.876	138.344	1.00	79.59	A	N
	ATOM	1606	CZ	ARG	301	-24.354	-39.813	138.602	1.00	79.96	A	C
	ATOM	1607	NH1	ARG	301	-24.557	-40.203	139.854	1.00	80.06	A	N
50	ATOM	1608	NH2	ARG	301	-25.057	-40.362	137.617	1.00	79.96	A	N
	ATOM	1609	C	ARG	301	-19.036	-37.568	135.678	1.00	76.98	A	C
	ATOM	1610	O	ARG	301	-18.188	-37.686	134.788	1.00	76.77	A	O
	ATOM	1611	N	ARG	302	-19.141	-38.399	136.713	1.00	77.23	A	N
	ATOM	1612	CA	ARG	302	-18.288	-39.563	136.920	1.00	77.33	A	C
	ATOM	1613	CB	ARG	302	-18.689	-40.250	138.232	1.00	77.94	A	C
	ATOM	1614	CG	ARG	302	-18.767	-39.306	139.425	1.00	79.00	A	C
55	ATOM	1615	CD	ARG	302	-19.352	-39.993	140.647	1.00	80.06	A	C
	ATOM	1616	NE	ARG	302	-19.619	-39.045	141.727	1.00	80.81	A	N

-197-

	ATOM	1617	CZ	ARG	302	-20.120	-39.375	142.915	1.00	81.28	A	C
	ATOM	1618	NH1	ARG	302	-20.414	-40.640	143.190	1.00	81.53	A	N
	ATOM	1619	NH2	ARG	302	-20.329	-38.437	143.830	1.00	81.32	A	N
5	ATOM	1620	C	ARG	302	-18.432	-40.541	135.748	1.00	76.86	A	C
	ATOM	1621	O	ARG	302	-19.245	-40.326	134.848	1.00	77.13	A	O
	ATOM	1622	N	PRO	303	-17.641	-41.627	135.740	1.00	76.19	A	N
	ATOM	1623	CD	PRO	303	-17.651	-42.598	134.632	1.00	76.11	A	C
	ATOM	1624	CA	PRO	303	-16.638	-41.999	136.747	1.00	75.35	A	C
10	ATOM	1625	CB	PRO	303	-16.150	-43.362	136.257	1.00	75.81	A	C
	ATOM	1626	CG	PRO	303	-16.298	-43.254	134.770	1.00	75.99	A	C
	ATOM	1627	C	PRO	303	-15.502	-40.983	136.888	1.00	74.26	A	C
	ATOM	1628	O	PRO	303	-14.879	-40.586	135.901	1.00	74.49	A	O
	ATOM	1629	N	ARG	304	-15.251	-40.562	138.125	1.00	72.62	A	N
15	ATOM	1630	CA	ARG	304	-14.193	-39.600	138.422	1.00	70.74	A	C
	ATOM	1631	CB	ARG	304	-13.927	-39.545	139.932	1.00	71.66	A	C
	ATOM	1632	CG	ARG	304	-13.223	-40.787	140.498	1.00	72.36	A	C
	ATOM	1633	CD	ARG	304	-14.164	-41.984	140.613	1.00	73.27	A	C
	ATOM	1634	NE	ARG	304	-13.466	-43.229	140.936	1.00	73.97	A	N
20	ATOM	1635	CZ	ARG	304	-12.741	-43.940	140.075	1.00	74.21	A	C
	ATOM	1636	NH1	ARG	304	-12.601	-43.543	138.817	1.00	74.26	A	N
	ATOM	1637	NH2	ARG	304	-12.154	-45.060	140.473	1.00	74.59	A	N
	ATOM	1638	C	ARG	304	-12.909	-40.014	137.716	1.00	68.87	A	C
	ATOM	1639	O	ARG	304	-12.746	-41.179	137.351	1.00	68.86	A	O
25	ATOM	1640	N	ASP	305	-11.995	-39.066	137.526	1.00	66.37	A	N
	ATOM	1641	CA	ASP	305	-10.727	-39.378	136.875	1.00	62.94	A	C
	ATOM	1642	CB	ASP	305	-10.978	-40.055	135.525	1.00	63.29	A	C
	ATOM	1643	CG	ASP	305	-9.704	-40.566	134.887	1.00	63.63	A	C
	ATOM	1644	OD1	ASP	305	-8.944	-41.283	135.570	1.00	63.64	A	O
30	ATOM	1645	OD2	ASP	305	-9.465	-40.259	133.701	1.00	64.48	A	O
	ATOM	1646	C	ASP	305	-9.804	-38.183	136.670	1.00	60.10	A	C
	ATOM	1647	O	ASP	305	-9.951	-37.428	135.704	1.00	59.69	A	O
	ATOM	1648	N	ARG	306	-8.855	-38.005	137.584	1.00	56.47	A	N
	ATOM	1649	CA	ARG	306	-7.896	-36.918	137.437	1.00	52.72	A	C
35	ATOM	1650	CB	ARG	306	-7.376	-36.424	138.792	1.00	54.11	A	C
	ATOM	1651	CG	ARG	306	-6.551	-35.137	138.659	1.00	55.62	A	C
	ATOM	1652	CD	ARG	306	-5.264	-35.152	139.480	1.00	57.19	A	C
	ATOM	1653	NE	ARG	306	-5.384	-34.423	140.743	1.00	58.88	A	N
	ATOM	1654	CZ	ARG	306	-4.358	-34.121	141.537	1.00	59.27	A	C
40	ATOM	1655	NH1	ARG	306	-3.125	-34.487	141.204	1.00	59.61	A	N
	ATOM	1656	NH2	ARG	306	-4.561	-33.443	142.662	1.00	59.29	A	N
	ATOM	1657	C	ARG	306	-6.721	-37.437	136.612	1.00	49.02	A	C
	ATOM	1658	O	ARG	306	-5.719	-36.750	136.448	1.00	49.06	A	O
	ATOM	1659	N	PHE	307	-6.857	-38.659	136.101	1.00	44.87	A	N
45	ATOM	1660	CA	PHE	307	-5.828	-39.299	135.288	1.00	40.64	A	C
	ATOM	1661	CB	PHE	307	-5.889	-40.819	135.477	1.00	39.73	A	C
	ATOM	1662	CG	PHE	307	-5.603	-41.275	136.880	1.00	39.02	A	C
	ATOM	1663	CD1	PHE	307	-4.295	-41.358	137.349	1.00	38.54	A	C
	ATOM	1664	CD2	PHE	307	-6.644	-41.615	137.738	1.00	38.66	A	C
50	ATOM	1665	CE1	PHE	307	-4.026	-41.774	138.650	1.00	38.12	A	C
	ATOM	1666	CE2	PHE	307	-6.385	-42.032	139.044	1.00	39.04	A	C
	ATOM	1667	CZ	PHE	307	-5.072	-42.112	139.499	1.00	38.17	A	C
	ATOM	1668	C	PHE	307	-5.976	-38.982	133.796	1.00	38.25	A	C
	ATOM	1669	O	PHE	307	-5.036	-39.160	133.026	1.00	36.74	A	O
55	ATOM	1670	N	LEU	308	-7.150	-38.504	133.391	1.00	35.76	A	N
	ATOM	1671	CA	LEU	308	-7.397	-38.212	131.984	1.00	33.41	A	C
	ATOM	1672	CB	LEU	308	-8.819	-37.672	131.792	1.00	33.07	A	C
	ATOM	1673	CG	LEU	308	-9.360	-37.618	130.351	1.00	33.17	A	C
	ATOM	1674	CD1	LEU	308	-8.779	-36.444	129.613	1.00	34.19	A	C

-198-

	ATOM	1675	CD2	LEU	308	-9.036	-38.913	129.623	1.00	31.34	A	C
	ATOM	1676	C	LEU	308	-6.389	-37.268	131.337	1.00	31.73	A	C
	ATOM	1677	O	LEU	308	-5.809	-37.601	130.306	1.00	30.35	A	O
5	ATOM	1678	N	TYR	309	-6.176	-36.097	131.928	1.00	29.96	A	N
	ATOM	1679	CA	TYR	309	-5.236	-35.149	131.346	1.00	28.55	A	C
	ATOM	1680	CB	TYR	309	-5.156	-33.865	132.171	1.00	28.94	A	C
	ATOM	1681	CG	TYR	309	-4.250	-32.828	131.543	1.00	29.27	A	C
	ATOM	1682	CD1	TYR	309	-4.567	-32.250	130.312	1.00	29.24	A	C
10	ATOM	1683	CE1	TYR	309	-3.719	-31.315	129.715	1.00	29.07	A	C
	ATOM	1684	CD2	TYR	309	-3.061	-32.443	132.162	1.00	29.31	A	C
	ATOM	1685	CE2	TYR	309	-2.209	-31.511	131.573	1.00	29.09	A	C
	ATOM	1686	CZ	TYR	309	-2.544	-30.955	130.353	1.00	28.97	A	C
	ATOM	1687	OH	TYR	309	-1.697	-30.049	129.766	1.00	29.80	A	O
15	ATOM	1688	C	TYR	309	-3.842	-35.738	131.198	1.00	27.07	A	C
	ATOM	1689	O	TYR	309	-3.204	-35.558	130.169	1.00	26.88	A	O
	ATOM	1690	N	ALA	310	-3.368	-36.436	132.225	1.00	25.89	A	N
	ATOM	1691	CA	ALA	310	-2.049	-37.051	132.169	1.00	25.16	A	C
	ATOM	1692	CB	ALA	310	-1.702	-37.690	133.512	1.00	24.32	A	C
20	ATOM	1693	C	ALA	310	-1.997	-38.096	131.046	1.00	24.96	A	C
	ATOM	1694	O	ALA	310	-1.023	-38.142	130.291	1.00	24.12	A	O
	ATOM	1695	N	LYS	311	-3.036	-38.930	130.940	1.00	23.97	A	N
	ATOM	1696	CA	LYS	311	-3.097	-39.938	129.881	1.00	24.13	A	C
	ATOM	1697	CB	LYS	311	-4.391	-40.752	129.960	1.00	25.00	A	C
25	ATOM	1698	CG	LYS	311	-4.473	-41.760	131.105	1.00	27.78	A	C
	ATOM	1699	CD	LYS	311	-5.831	-42.472	131.058	1.00	29.79	A	C
	ATOM	1700	CE	LYS	311	-6.089	-43.328	132.285	1.00	31.20	A	C
	ATOM	1701	NZ	LYS	311	-7.505	-43.836	132.302	1.00	33.50	A	N
	ATOM	1702	C	LYS	311	-3.031	-39.268	128.508	1.00	23.70	A	C
30	ATOM	1703	O	LYS	311	-2.430	-39.806	127.583	1.00	23.05	A	O
	ATOM	1704	N	LEU	312	-3.651	-38.098	128.378	1.00	22.94	A	N
	ATOM	1705	CA	LEU	312	-3.643	-37.380	127.113	1.00	23.55	A	C
	ATOM	1706	CB	LEU	312	-4.656	-36.230	127.143	1.00	24.36	A	C
	ATOM	1707	CG	LEU	312	-6.128	-36.661	127.073	1.00	25.69	A	C
35	ATOM	1708	CD1	LEU	312	-7.026	-35.447	126.879	1.00	24.81	A	C
	ATOM	1709	CD2	LEU	312	-6.312	-37.629	125.910	1.00	26.15	A	C
	ATOM	1710	C	LEU	312	-2.248	-36.860	126.748	1.00	23.28	A	C
	ATOM	1711	O	LEU	312	-1.859	-36.888	125.580	1.00	22.28	A	O
	ATOM	1712	N	LEU	313	-1.498	-36.374	127.733	1.00	22.16	A	N
40	ATOM	1713	CA	LEU	313	-0.145	-35.905	127.460	1.00	22.07	A	C
	ATOM	1714	CB	LEU	313	0.454	-35.225	128.694	1.00	21.00	A	C
	ATOM	1715	CG	LEU	313	-0.202	-33.891	129.064	1.00	21.22	A	C
	ATOM	1716	CD1	LEU	313	0.485	-33.316	130.284	1.00	20.26	A	C
	ATOM	1717	CD2	LEU	313	-0.115	-32.920	127.886	1.00	18.10	A	C
45	ATOM	1718	C	LEU	313	0.681	-37.131	127.059	1.00	22.48	A	C
	ATOM	1719	O	LEU	313	1.512	-37.068	126.152	1.00	22.20	A	O
	ATOM	1720	N	GLY	314	0.434	-38.251	127.733	1.00	22.89	A	N
	ATOM	1721	CA	GLY	314	1.131	-39.479	127.402	1.00	23.30	A	C
	ATOM	1722	C	GLY	314	0.860	-39.842	125.949	1.00	23.94	A	C
	ATOM	1723	O	GLY	314	1.782	-40.168	125.200	1.00	24.54	A	O
50	ATOM	1724	N	LEU	315	-0.410	-39.779	125.549	1.00	23.59	A	N
	ATOM	1725	CA	LEU	315	-0.807	-40.092	124.182	1.00	22.89	A	C
	ATOM	1726	CB	LEU	315	-2.336	-40.134	124.070	1.00	23.44	A	C
	ATOM	1727	CG	LEU	315	-2.961	-41.398	124.681	1.00	23.97	A	C
	ATOM	1728	CD1	LEU	315	-4.465	-41.270	124.742	1.00	23.92	A	C
55	ATOM	1729	CD2	LEU	315	-2.566	-42.613	123.854	1.00	23.72	A	C
	ATOM	1730	C	LEU	315	-0.221	-39.115	123.167	1.00	22.47	A	C
	ATOM	1731	O	LEU	315	0.094	-39.505	122.044	1.00	22.11	A	O
	ATOM	1732	N	LEU	316	-0.072	-37.849	123.544	1.00	22.35	A	N

-199-

5	ATOM	1733	CA	LEU	316	0.524	-36.882	122.626	1.00	22.93	A	C
	ATOM	1734	CB	LEU	316	0.454	-35.465	123.194	1.00	23.82	A	C
	ATOM	1735	CG	LEU	316	-0.934	-34.817	123.164	1.00	25.69	A	C
	ATOM	1736	CD1	LEU	316	-0.879	-33.440	123.802	1.00	25.97	A	C
	ATOM	1737	CD2	LEU	316	-1.418	-34.720	121.722	1.00	26.87	A	C
10	ATOM	1738	C	LEU	316	1.977	-37.273	122.401	1.00	23.05	A	C
	ATOM	1739	O	LEU	316	2.496	-37.162	121.290	1.00	23.13	A	O
	ATOM	1740	N	ALA	317	2.624	-37.741	123.464	1.00	22.68	A	N
	ATOM	1741	CA	ALA	317	4.009	-38.169	123.392	1.00	23.73	A	C
	ATOM	1742	CB	ALA	317	4.560	-38.439	124.804	1.00	23.13	A	C
15	ATOM	1743	C	ALA	317	4.111	-39.426	122.536	1.00	23.75	A	C
	ATOM	1744	O	ALA	317	5.043	-39.567	121.759	1.00	22.15	A	O
	ATOM	1745	N	GLU	318	3.150	-40.334	122.667	1.00	24.36	A	N
	ATOM	1746	CA	GLU	318	3.183	-41.562	121.881	1.00	26.08	A	C
	ATOM	1747	CB	GLU	318	2.115	-42.543	122.362	1.00	28.21	A	C
20	ATOM	1748	CG	GLU	318	2.116	-43.831	121.566	1.00	32.51	A	C
	ATOM	1749	CD	GLU	318	1.632	-45.004	122.375	1.00	35.59	A	C
	ATOM	1750	OE1	GLU	318	0.410	-45.114	122.604	1.00	36.82	A	O
	ATOM	1751	OE2	GLU	318	2.488	-45.811	122.796	1.00	38.53	A	O
	ATOM	1752	C	GLU	318	2.997	-41.300	120.391	1.00	25.72	A	C
25	ATOM	1753	O	GLU	318	3.641	-41.929	119.557	1.00	24.88	A	O
	ATOM	1754	N	LEU	319	2.101	-40.375	120.068	1.00	25.55	A	N
	ATOM	1755	CA	LEU	319	1.832	-40.001	118.684	1.00	25.73	A	C
	ATOM	1756	CB	LEU	319	0.684	-38.994	118.652	1.00	24.34	A	C
	ATOM	1757	CG	LEU	319	0.123	-38.538	117.311	1.00	24.57	A	C
30	ATOM	1758	CD1	LEU	319	-0.173	-39.730	116.426	1.00	21.78	A	C
	ATOM	1759	CD2	LEU	319	-1.131	-37.713	117.576	1.00	23.45	A	C
	ATOM	1760	C	LEU	319	3.112	-39.395	118.103	1.00	26.16	A	C
	ATOM	1761	O	LEU	319	3.389	-39.500	116.907	1.00	26.27	A	O
	ATOM	1762	N	ARG	320	3.889	-38.757	118.969	1.00	26.63	A	N
35	ATOM	1763	CA	ARG	320	5.159	-38.169	118.587	1.00	27.47	A	C
	ATOM	1764	CB	ARG	320	5.750	-37.430	119.786	1.00	29.62	A	C
	ATOM	1765	CG	ARG	320	6.936	-36.574	119.463	1.00	32.70	A	C
	ATOM	1766	CD	ARG	320	6.505	-35.319	118.741	1.00	35.19	A	C
	ATOM	1767	NE	ARG	320	7.665	-34.554	118.307	1.00	36.76	A	N
40	ATOM	1768	CZ	ARG	320	7.899	-33.287	118.624	1.00	37.53	A	C
	ATOM	1769	NH1	ARG	320	7.054	-32.609	119.389	1.00	37.83	A	N
	ATOM	1770	NH2	ARG	320	8.993	-32.697	118.166	1.00	39.80	A	N
	ATOM	1771	C	ARG	320	6.081	-39.326	118.169	1.00	26.95	A	C
	ATOM	1772	O	ARG	320	6.849	-39.209	117.209	1.00	27.09	A	O
45	ATOM	1773	N	SER	321	5.996	-40.441	118.898	1.00	25.51	A	N
	ATOM	1774	CA	SER	321	6.790	-41.638	118.603	1.00	25.26	A	C
	ATOM	1775	CB	SER	321	6.577	-42.720	119.661	1.00	24.40	A	C
	ATOM	1776	OG	SER	321	7.275	-42.419	120.843	1.00	26.98	A	O
	ATOM	1777	C	SER	321	6.377	-42.210	117.261	1.00	24.22	A	C
50	ATOM	1778	O	SER	321	7.219	-42.588	116.450	1.00	23.84	A	O
	ATOM	1779	N	ILE	322	5.069	-42.293	117.051	1.00	23.23	A	N
	ATOM	1780	CA	ILE	322	4.521	-42.802	115.810	1.00	23.56	A	C
	ATOM	1781	CB	ILE	322	2.979	-42.784	115.876	1.00	23.28	A	C
	ATOM	1782	CG2	ILE	322	2.377	-42.970	114.484	1.00	22.26	A	C
55	ATOM	1783	CG1	ILE	322	2.513	-43.873	116.855	1.00	22.75	A	C
	ATOM	1784	CD1	ILE	322	1.021	-43.879	117.140	1.00	21.11	A	C
	ATOM	1785	C	ILE	322	5.024	-41.955	114.639	1.00	24.10	A	C
	ATOM	1786	O	ILE	322	5.387	-42.489	113.590	1.00	23.74	A	O
	ATOM	1787	N	ASN	323	5.055	-40.637	114.826	1.00	24.50	A	N
	ATOM	1788	CA	ASN	323	5.523	-39.724	113.787	1.00	25.76	A	C
	ATOM	1789	CB	ASN	323	5.477	-38.280	114.295	1.00	27.72	A	C
	ATOM	1790	CG	ASN	323	5.909	-37.271	113.244	1.00	30.34	A	C

-200-

	ATOM	1791	OD1	ASN	323	6.870	-37.489	112.509	1.00	33.18	A	O
	ATOM	1792	ND2	ASN	323	5.215	-36.148	113.189	1.00	31.75	A	N
	ATOM	1793	C	ASN	323	6.953	-40.100	113.408	1.00	25.95	A	C
5	ATOM	1794	O	ASN	323	7.265	-40.282	112.236	1.00	25.34	A	O
	ATOM	1795	N	GLU	324	7.817	-40.232	114.410	1.00	26.65	A	N
	ATOM	1796	CA	GLU	324	9.208	-40.597	114.173	1.00	27.58	A	C
	ATOM	1797	CB	GLU	324	9.994	-40.535	115.482	1.00	30.21	A	C
	ATOM	1798	CG	GLU	324	9.920	-39.180	116.165	1.00	34.60	A	C
10	ATOM	1799	CD	GLU	324	10.646	-39.163	117.490	1.00	37.84	A	C
	ATOM	1800	OE1	GLU	324	10.494	-40.138	118.258	1.00	39.66	A	O
	ATOM	1801	OE2	GLU	324	11.359	-38.173	117.770	1.00	39.51	A	O
	ATOM	1802	C	GLU	324	9.343	-41.988	113.549	1.00	26.74	A	C
	ATOM	1803	O	GLU	324	10.238	-42.221	112.740	1.00	26.19	A	O
15	ATOM	1804	N	ALA	325	8.464	-42.914	113.923	1.00	25.09	A	N
	ATOM	1805	CA	ALA	325	8.517	-44.258	113.359	1.00	25.00	A	C
	ATOM	1806	CB	ALA	325	7.619	-45.209	114.153	1.00	24.73	A	C
	ATOM	1807	C	ALA	325	8.111	-44.238	111.878	1.00	24.89	A	C
	ATOM	1808	O	ALA	325	8.561	-45.073	111.093	1.00	25.47	A	O
20	ATOM	1809	N	TYR	326	7.250	-43.297	111.502	1.00	23.96	A	N
	ATOM	1810	CA	TYR	326	6.845	-43.145	110.106	1.00	23.70	A	C
	ATOM	1811	CB	TYR	326	5.856	-41.988	109.952	1.00	22.03	A	C
	ATOM	1812	CG	TYR	326	4.413	-42.402	109.901	1.00	21.43	A	C
	ATOM	1813	CD1	TYR	326	3.922	-43.180	108.848	1.00	20.69	A	C
25	ATOM	1814	CE1	TYR	326	2.571	-43.541	108.787	1.00	19.55	A	C
	ATOM	1815	CD2	TYR	326	3.521	-41.996	110.897	1.00	21.09	A	C
	ATOM	1816	CE2	TYR	326	2.175	-42.348	110.845	1.00	20.21	A	C
	ATOM	1817	CZ	TYR	326	1.707	-43.117	109.791	1.00	20.21	A	C
	ATOM	1818	OH	TYR	326	0.374	-43.439	109.749	1.00	19.33	A	O
30	ATOM	1819	C	TYR	326	8.093	-42.827	109.280	1.00	24.16	A	C
	ATOM	1820	O	TYR	326	8.276	-43.360	108.196	1.00	23.33	A	O
	ATOM	1821	N	GLY	327	8.933	-41.936	109.802	1.00	25.27	A	N
	ATOM	1822	CA	GLY	327	10.158	-41.563	109.116	1.00	26.47	A	C
	ATOM	1823	C	GLY	327	11.054	-42.765	108.912	1.00	27.58	A	C
35	ATOM	1824	O	GLY	327	11.633	-42.937	107.848	1.00	27.44	A	O
	ATOM	1825	N	TYR	328	11.176	-43.601	109.938	1.00	29.10	A	N
	ATOM	1826	CA	TYR	328	11.992	-44.801	109.838	1.00	30.30	A	C
	ATOM	1827	CB	TYR	328	12.018	-45.537	111.182	1.00	31.95	A	C
	ATOM	1828	CG	TYR	328	12.753	-46.859	111.127	1.00	33.79	A	C
40	ATOM	1829	CD1	TYR	328	14.129	-46.930	111.361	1.00	35.24	A	C
	ATOM	1830	CE1	TYR	328	14.819	-48.144	111.242	1.00	36.06	A	C
	ATOM	1831	CD2	TYR	328	12.084	-48.032	110.778	1.00	34.19	A	C
	ATOM	1832	CE2	TYR	328	12.760	-49.243	110.652	1.00	35.21	A	C
	ATOM	1833	CZ	TYR	328	14.126	-49.293	110.884	1.00	36.45	A	C
45	ATOM	1834	OH	TYR	328	14.797	-50.489	110.736	1.00	37.83	A	O
	ATOM	1835	C	TYR	328	11.411	-45.722	108.758	1.00	30.82	A	C
	ATOM	1836	O	TYR	328	12.145	-46.306	107.966	1.00	30.88	A	O
	ATOM	1837	N	GLN	329	10.088	-45.852	108.737	1.00	31.03	A	N
	ATOM	1838	CA	GLN	329	9.412	-46.699	107.759	1.00	31.18	A	C
50	ATOM	1839	CB	GLN	329	7.902	-46.700	108.011	1.00	29.87	A	C
	ATOM	1840	CG	GLN	329	7.486	-47.228	109.377	1.00	30.38	A	C
	ATOM	1841	CD	GLN	329	7.716	-48.717	109.523	1.00	31.26	A	C
	ATOM	1842	OE1	GLN	329	8.533	-49.168	110.338	1.00	30.58	A	O
	ATOM	1843	NE2	GLN	329	6.995	-49.496	108.729	1.00	30.24	A	N
55	ATOM	1844	C	GLN	329	9.688	-46.220	106.338	1.00	31.84	A	C
	ATOM	1845	O	GLN	329	10.002	-47.017	105.457	1.00	31.67	A	O
	ATOM	1846	N	ILE	330	9.565	-44.916	106.118	1.00	32.78	A	N
	ATOM	1847	CA	ILE	330	9.796	-44.336	104.800	1.00	34.51	A	C
	ATOM	1848	CB	ILE	330	9.423	-42.833	104.798	1.00	34.57	A	C

-201-

	ATOM	1849	CG2	ILE	330	10.061	-42.113	103.613	1.00	34.87	A	C
	ATOM	1850	CG1	ILE	330	7.900	-42.697	104.752	1.00	34.64	A	C
	ATOM	1851	CD1	ILE	330	7.407	-41.267	104.779	1.00	35.62	A	C
5	ATOM	1852	C	ILE	330	11.231	-44.519	104.300	1.00	35.74	A	C
	ATOM	1853	O	ILE	330	11.467	-44.599	103.094	1.00	34.91	A	O
	ATOM	1854	N	GLN	331	12.179	-44.604	105.228	1.00	37.46	A	N
	ATOM	1855	CA	GLN	331	13.586	-44.776	104.882	1.00	39.69	A	C
	ATOM	1856	CB	GLN	331	14.473	-44.235	105.999	1.00	42.13	A	C
10	ATOM	1857	CG	GLN	331	14.507	-42.735	106.134	1.00	44.67	A	C
	ATOM	1858	CD	GLN	331	15.164	-42.325	107.428	1.00	47.11	A	C
	ATOM	1859	OE1	GLN	331	16.202	-42.870	107.806	1.00	48.26	A	O
	ATOM	1860	NE2	GLN	331	14.565	-41.362	108.120	1.00	48.66	A	N
	ATOM	1861	C	GLN	331	14.010	-46.211	104.613	1.00	39.80	A	C
15	ATOM	1862	O	GLN	331	14.843	-46.463	103.749	1.00	40.44	A	O
	ATOM	1863	N	HIS	332	13.446	-47.155	105.351	1.00	39.86	A	N
	ATOM	1864	CA	HIS	332	13.839	-48.546	105.187	1.00	40.67	A	C
	ATOM	1865	CB	HIS	332	14.048	-49.161	106.571	1.00	42.81	A	C
	ATOM	1866	CG	HIS	332	15.172	-48.524	107.331	1.00	46.28	A	C
20	ATOM	1867	CD2	HIS	332	15.209	-47.399	108.086	1.00	47.01	A	C
	ATOM	1868	ND1	HIS	332	16.466	-48.992	107.275	1.00	47.57	A	N
	ATOM	1869	CE1	HIS	332	17.256	-48.181	107.961	1.00	47.73	A	C
	ATOM	1870	NE2	HIS	332	16.518	-47.208	108.461	1.00	48.10	A	N
	ATOM	1871	C	HIS	332	12.928	-49.422	104.337	1.00	39.76	A	C
25	ATOM	1872	O	HIS	332	13.241	-50.587	104.082	1.00	39.61	A	O
	ATOM	1873	N	ILE	333	11.810	-48.871	103.882	1.00	38.23	A	N
	ATOM	1874	CA	ILE	333	10.900	-49.647	103.055	1.00	37.05	A	C
	ATOM	1875	CB	ILE	333	9.567	-49.887	103.779	1.00	36.60	A	C
	ATOM	1876	CG2	ILE	333	8.618	-50.652	102.878	1.00	36.04	A	C
30	ATOM	1877	CG1	ILE	333	9.824	-50.680	105.066	1.00	37.04	A	C
	ATOM	1878	CD1	ILE	333	8.620	-50.826	105.963	1.00	36.04	A	C
	ATOM	1879	C	ILE	333	10.656	-48.967	101.713	1.00	36.44	A	C
	ATOM	1880	O	ILE	333	9.841	-48.056	101.599	1.00	36.09	A	O
	ATOM	1881	N	GLN	334	11.394	-49.424	100.707	1.00	35.60	A	N
35	ATOM	1882	CA	GLN	334	11.309	-48.909	99.345	1.00	35.11	A	C
	ATOM	1883	CB	GLN	334	12.172	-49.788	98.427	1.00	37.05	A	C
	ATOM	1884	CG	GLN	334	12.764	-49.113	97.192	1.00	40.94	A	C
	ATOM	1885	CD	GLN	334	11.771	-48.947	96.055	1.00	43.49	A	C
	ATOM	1886	OE1	GLN	334	10.952	-48.031	96.060	1.00	45.60	A	O
40	ATOM	1887	NE2	GLN	334	11.838	-49.846	95.071	1.00	44.60	A	N
	ATOM	1888	C	GLN	334	9.851	-48.925	98.888	1.00	33.48	A	C
	ATOM	1889	O	GLN	334	9.151	-49.929	99.036	1.00	32.53	A	O
	ATOM	1890	N	GLY	335	9.388	-47.801	98.353	1.00	32.61	A	N
	ATOM	1891	CA	GLY	335	8.019	-47.724	97.879	1.00	31.27	A	C
45	ATOM	1892	C	GLY	335	7.029	-47.059	98.816	1.00	30.52	A	C
	ATOM	1893	O	GLY	335	6.029	-46.519	98.357	1.00	29.45	A	O
	ATOM	1894	N	LEU	336	7.289	-47.091	100.122	1.00	30.35	A	N
	ATOM	1895	CA	LEU	336	6.371	-46.474	101.073	1.00	30.47	A	C
	ATOM	1896	CB	LEU	336	6.837	-46.683	102.515	1.00	30.60	A	C
	ATOM	1897	CG	LEU	336	6.505	-47.973	103.265	1.00	31.59	A	C
50	ATOM	1898	CD1	LEU	336	6.881	-47.777	104.731	1.00	32.05	A	C
	ATOM	1899	CD2	LEU	336	5.027	-48.308	103.153	1.00	31.01	A	C
	ATOM	1900	C	LEU	336	6.186	-44.983	100.845	1.00	30.50	A	C
	ATOM	1901	O	LEU	336	5.066	-44.487	100.891	1.00	29.66	A	O
55	ATOM	1902	N	SER	337	7.283	-44.271	100.603	1.00	31.26	A	N
	ATOM	1903	CA	SER	337	7.224	-42.829	100.395	1.00	32.62	A	C
	ATOM	1904	CB	SER	337	8.628	-42.267	100.141	1.00	33.56	A	C
	ATOM	1905	OG	SER	337	9.184	-42.777	98.943	1.00	35.00	A	O
	ATOM	1906	C	SER	337	6.286	-42.419	99.263	1.00	32.68	A	C

-202-

	ATOM	1907	O	SER	337	5.792	-41.300	99.246	1.00	33.22	A	O
	ATOM	1908	N	ALA	338	6.030	-43.321	98.324	1.00	33.04	A	N
	ATOM	1909	CA	ALA	338	5.133	-43.016	97.218	1.00	33.69	A	C
5	ATOM	1910	CB	ALA	338	5.072	-44.199	96.257	1.00	33.20	A	C
	ATOM	1911	C	ALA	338	3.723	-42.669	97.711	1.00	34.44	A	C
	ATOM	1912	O	ALA	338	2.979	-41.952	97.032	1.00	34.62	A	O
	ATOM	1913	N	MET	339	3.348	-43.186	98.879	1.00	34.28	A	N
	ATOM	1914	CA	MET	339	2.024	-42.906	99.422	1.00	35.53	A	C
10	ATOM	1915	CB	MET	339	1.604	-44.003	100.400	1.00	31.99	A	C
	ATOM	1916	CG	MET	339	1.203	-45.292	99.701	1.00	29.56	A	C
	ATOM	1917	SD	MET	339	0.803	-46.628	100.838	1.00	26.76	A	S
	ATOM	1918	CE	MET	339	2.486	-47.154	101.313	1.00	25.89	A	C
	ATOM	1919	C	MET	339	1.956	-41.537	100.086	1.00	38.11	A	C
15	ATOM	1920	O	MET	339	0.883	-41.074	100.475	1.00	38.51	A	O
	ATOM	1921	N	MET	340	3.108	-40.891	100.217	1.00	41.19	A	N
	ATOM	1922	CA	MET	340	3.162	-39.564	100.792	1.00	45.17	A	C
	ATOM	1923	CB	MET	340	3.933	-39.576	102.108	1.00	45.06	A	C
	ATOM	1924	CG	MET	340	3.761	-38.294	102.892	1.00	45.91	A	C
20	ATOM	1925	SD	MET	340	2.006	-37.937	103.173	1.00	46.05	A	S
	ATOM	1926	CE	MET	340	1.556	-37.032	101.643	1.00	45.26	A	C
	ATOM	1927	C	MET	340	3.848	-38.636	99.793	1.00	48.30	A	C
	ATOM	1928	O	MET	340	4.965	-38.182	100.023	1.00	48.09	A	O
	ATOM	1929	N	PRO	341	3.180	-38.348	98.662	1.00	51.89	A	N
25	ATOM	1930	CD	PRO	341	1.818	-38.785	98.307	1.00	52.61	A	C
	ATOM	1931	CA	PRO	341	3.725	-37.474	97.616	1.00	55.17	A	C
	ATOM	1932	CB	PRO	341	2.552	-37.321	96.649	1.00	54.46	A	C
	ATOM	1933	CG	PRO	341	1.812	-38.613	96.810	1.00	53.80	A	C
	ATOM	1934	C	PRO	341	4.201	-36.129	98.151	1.00	58.43	A	C
30	ATOM	1935	O	PRO	341	5.399	-35.838	98.177	1.00	58.94	A	O
	ATOM	1936	N	LEU	342	3.244	-35.312	98.573	1.00	61.89	A	N
	ATOM	1937	CA	LEU	342	3.538	-33.993	99.108	1.00	65.33	A	C
	ATOM	1938	CB	LEU	342	2.297	-33.094	99.015	1.00	65.46	A	C
	ATOM	1939	CG	LEU	342	1.863	-32.488	97.675	1.00	65.98	A	C
35	ATOM	1940	CD1	LEU	342	1.636	-33.558	96.613	1.00	66.50	A	C
	ATOM	1941	CD2	LEU	342	0.586	-31.702	97.907	1.00	66.63	A	C
	ATOM	1942	C	LEU	342	3.956	-34.121	100.563	1.00	67.54	A	C
	ATOM	1943	O	LEU	342	3.808	-35.183	101.167	1.00	67.71	A	O
	ATOM	1944	N	LEU	343	4.490	-33.033	101.110	1.00	70.31	A	N
40	ATOM	1945	CA	LEU	343	4.909	-32.986	102.505	1.00	73.10	A	C
	ATOM	1946	CB	LEU	343	3.669	-32.854	103.401	1.00	73.06	A	C
	ATOM	1947	CG	LEU	343	3.783	-32.206	104.783	1.00	73.13	A	C
	ATOM	1948	CD1	LEU	343	4.851	-32.903	105.615	1.00	73.35	A	C
	ATOM	1949	CD2	LEU	343	4.111	-30.733	104.613	1.00	73.19	A	C
45	ATOM	1950	C	LEU	343	5.712	-34.220	102.919	1.00	75.17	A	C
	ATOM	1951	O	LEU	343	5.138	-35.263	103.242	1.00	75.75	A	O
	ATOM	1952	N	GLN	344	7.037	-34.095	102.908	1.00	77.19	A	N
	ATOM	1953	CA	GLN	344	7.928	-35.185	103.303	1.00	79.02	A	C
	ATOM	1954	CB	GLN	344	7.588	-36.483	102.552	1.00	79.26	A	C
50	ATOM	1955	CG	GLN	344	7.934	-36.476	101.062	1.00	79.55	A	C
	ATOM	1956	CD	GLN	344	8.169	-37.876	100.495	1.00	79.92	A	C
	ATOM	1957	OE1	GLN	344	8.352	-38.044	99.288	1.00	80.00	A	O
	ATOM	1958	NE2	GLN	344	8.173	-38.884	101.366	1.00	79.76	A	N
	ATOM	1959	C	GLN	344	9.386	-34.823	103.034	1.00	80.26	A	C
55	ATOM	1960	O	GLN	344	9.691	-33.714	102.587	1.00	80.47	A	O
	ATOM	1961	N	GLU	345	10.283	-35.766	103.314	1.00	81.48	A	N
	ATOM	1962	CA	GLU	345	11.710	-35.565	103.093	1.00	82.57	A	C
	ATOM	1963	CB	GLU	345	12.522	-36.275	104.182	1.00	83.18	A	C
	ATOM	1964	CG	GLU	345	12.229	-35.802	105.598	1.00	84.08	A	C

-203-

5	ATOM	1965	CD	GLU	345	13.093	-36.500	106.634	1.00	84.62	A	C
	ATOM	1966	OE1	GLU	345	13.032	-37.746	106.722	1.00	85.08	A	O
	ATOM	1967	OE2	GLU	345	13.834	-35.801	107.359	1.00	84.92	A	O
	ATOM	1968	C	GLU	345	12.106	-36.112	101.721	1.00	82.85	A	C
	ATOM	1969	O	GLU	345	13.062	-36.916	101.657	1.00	83.15	A	O
10	ATOM	1970	OXT	GLU	345	11.457	-35.728	100.723	1.00	83.01	A	O
	TER	1971		GLU	345						A	
	ATOM	1972	CB	PRO	103	12.922	-89.522	143.199	1.00	81.05	B	C
	ATOM	1973	CG	PRO	103	13.639	-89.140	144.492	1.00	81.13	B	C
	ATOM	1974	C	PRO	103	13.827	-89.814	140.872	1.00	80.76	B	C
15	ATOM	1975	O	PRO	103	13.218	-88.817	140.479	1.00	80.92	B	O
	ATOM	1976	N	PRO	103	15.298	-89.351	142.841	1.00	81.13	B	N
	ATOM	1977	CD	PRO	103	14.976	-88.538	144.028	1.00	81.18	B	C
	ATOM	1978	CA	PRO	103	14.080	-90.046	142.362	1.00	80.95	B	C
	ATOM	1979	N	VAL	104	14.299	-90.742	140.047	1.00	80.28	B	N
20	ATOM	1980	CA	VAL	104	14.125	-90.648	138.601	1.00	79.68	B	C
	ATOM	1981	CB	VAL	104	15.488	-90.651	137.868	1.00	79.97	B	C
	ATOM	1982	CG1	VAL	104	16.297	-89.424	138.267	1.00	80.04	B	C
	ATOM	1983	CG2	VAL	104	16.254	-91.933	138.186	1.00	79.80	B	C
	ATOM	1984	C	VAL	104	13.296	-91.823	138.096	1.00	78.96	B	C
25	ATOM	1985	O	VAL	104	13.242	-92.872	138.740	1.00	79.04	B	O
	ATOM	1986	N	GLN	105	12.654	-91.649	136.943	1.00	77.77	B	N
	ATOM	1987	CA	GLN	105	11.830	-92.710	136.373	1.00	76.25	B	C
	ATOM	1988	CB	GLN	105	10.461	-92.159	135.952	1.00	76.99	B	C
	ATOM	1989	CG	GLN	105	9.447	-93.249	135.604	1.00	77.64	B	C
30	ATOM	1990	CD	GLN	105	8.032	-92.718	135.433	1.00	78.06	B	C
	ATOM	1991	OE1	GLN	105	7.534	-91.960	136.268	1.00	78.05	B	O
	ATOM	1992	NE2	GLN	105	7.371	-93.130	134.355	1.00	77.95	B	N
	ATOM	1993	C	GLN	105	12.495	-93.407	135.185	1.00	74.64	B	C
	ATOM	1994	O	GLN	105	12.485	-94.634	135.110	1.00	74.66	B	O
35	ATOM	1995	N	LEU	106	13.067	-92.618	134.273	1.00	72.54	B	N
	ATOM	1996	CA	LEU	106	13.747	-93.115	133.070	1.00	70.12	B	C
	ATOM	1997	CB	LEU	106	15.259	-92.860	133.160	1.00	70.25	B	C
	ATOM	1998	CG	LEU	106	15.813	-91.432	133.205	1.00	70.18	B	C
	ATOM	1999	CD1	LEU	106	15.723	-90.881	134.616	1.00	70.47	B	C
40	ATOM	2000	CD2	LEU	106	17.267	-91.442	132.752	1.00	69.72	B	C
	ATOM	2001	C	LEU	106	13.521	-94.596	132.761	1.00	68.42	B	C
	ATOM	2002	O	LEU	106	14.449	-95.402	132.853	1.00	68.15	B	O
	ATOM	2003	N	SER	107	12.295	-94.949	132.382	1.00	66.23	B	N
	ATOM	2004	CA	SER	107	11.955	-96.333	132.064	1.00	63.76	B	C
45	ATOM	2005	CB	SER	107	10.469	-96.441	131.721	1.00	63.69	B	C
	ATOM	2006	OG	SER	107	10.152	-97.713	131.185	1.00	63.42	B	O
	ATOM	2007	C	SER	107	12.782	-96.865	130.904	1.00	62.28	B	C
	ATOM	2008	O	SER	107	13.328	-96.097	130.117	1.00	62.13	B	O
	ATOM	2009	N	LYS	108	12.878	-98.187	130.806	1.00	60.42	B	N
50	ATOM	2010	CA	LYS	108	13.633	-98.817	129.733	1.00	58.34	B	C
	ATOM	2011	CB	LYS	108	13.706	-100.328	129.957	1.00	59.09	B	C
	ATOM	2012	CG	LYS	108	14.716	-101.043	129.078	1.00	59.82	B	C
	ATOM	2013	CD	LYS	108	16.139	-100.630	129.430	1.00	61.01	B	C
	ATOM	2014	CE	LYS	108	17.167	-101.382	128.589	1.00	61.73	B	C
55	ATOM	2015	NZ	LYS	108	18.572	-101.025	128.958	1.00	62.47	B	N
	ATOM	2016	C	LYS	108	12.929	-98.524	128.415	1.00	56.63	B	C
	ATOM	2017	O	LYS	108	13.524	-97.970	127.491	1.00	56.15	B	O
	ATOM	2018	N	GLU	109	11.654	-98.895	128.342	1.00	54.51	B	N
	ATOM	2019	CA	GLU	109	10.846	-98.673	127.148	1.00	52.68	B	C
55	ATOM	2020	CB	GLU	109	9.464	-99.323	127.297	1.00	53.23	B	C
	ATOM	2021	CG	GLU	109	9.004	-99.560	128.730	1.00	54.59	B	C
	ATOM	2022	CD	GLU	109	9.624	-100.809	129.340	1.00	55.04	B	C

-204-

	ATOM	2023	OE1	GLU	109	9.379	-101.914	128.809	1.00	55.28	B	O
	ATOM	2024	OE2	GLU	109	10.359	-100.685	130.343	1.00	55.07	B	O
	ATOM	2025	C	GLU	109	10.684	-97.191	126.819	1.00	50.98	B	C
5	ATOM	2026	O	GLU	109	10.487	-96.832	125.662	1.00	50.38	B	O
	ATOM	2027	N	GLN	110	10.755	-96.333	127.832	1.00	49.17	B	N
	ATOM	2028	CA	GLN	110	10.636	-94.901	127.607	1.00	47.33	B	C
	ATOM	2029	CB	GLN	110	10.418	-94.156	128.926	1.00	47.12	B	C
	ATOM	2030	CG	GLN	110	9.089	-94.471	129.606	1.00	47.16	B	C
10	ATOM	2031	CD	GLN	110	8.874	-93.656	130.870	1.00	47.26	B	C
	ATOM	2032	OE1	GLN	110	9.767	-93.545	131.711	1.00	46.64	B	O
	ATOM	2033	NE2	GLN	110	7.682	-93.086	131.014	1.00	47.72	B	N
	ATOM	2034	C	GLN	110	11.896	-94.386	126.921	1.00	46.46	B	C
	ATOM	2035	O	GLN	110	11.815	-93.558	126.018	1.00	45.75	B	O
15	ATOM	2036	N	GLU	111	13.061	-94.871	127.343	1.00	45.39	B	N
	ATOM	2037	CA	GLU	111	14.306	-94.441	126.714	1.00	44.94	B	C
	ATOM	2038	CB	GLU	111	15.526	-95.026	127.436	1.00	46.33	B	C
	ATOM	2039	CG	GLU	111	15.591	-94.724	128.924	1.00	48.97	B	C
	ATOM	2040	CD	GLU	111	17.005	-94.789	129.479	1.00	50.99	B	C
20	ATOM	2041	OE1	GLU	111	17.745	-93.789	129.335	1.00	51.59	B	O
	ATOM	2042	OE2	GLU	111	17.378	-95.840	130.049	1.00	51.77	B	O
	ATOM	2043	C	GLU	111	14.292	-94.918	125.262	1.00	43.27	B	C
	ATOM	2044	O	GLU	111	14.768	-94.227	124.362	1.00	42.84	B	O
	ATOM	2045	N	GLU	112	13.735	-96.107	125.050	1.00	41.39	B	N
25	ATOM	2046	CA	GLU	112	13.627	-96.696	123.724	1.00	39.73	B	C
	ATOM	2047	CB	GLU	112	13.040	-98.104	123.833	1.00	40.89	B	C
	ATOM	2048	CG	GLU	112	12.809	-98.801	122.500	1.00	43.06	B	C
	ATOM	2049	CD	GLU	112	14.047	-98.808	121.624	1.00	44.55	B	C
	ATOM	2050	OE1	GLU	112	15.139	-99.130	122.139	1.00	45.11	B	O
30	ATOM	2051	OE2	GLU	112	13.927	-98.497	120.419	1.00	46.10	B	O
	ATOM	2052	C	GLU	112	12.733	-95.825	122.844	1.00	38.09	B	C
	ATOM	2053	O	GLU	112	13.030	-95.594	121.666	1.00	37.26	B	O
	ATOM	2054	N	LEU	113	11.638	-95.349	123.430	1.00	35.31	B	N
	ATOM	2055	CA	LEU	113	10.691	-94.500	122.729	1.00	33.09	B	C
35	ATOM	2056	CB	LEU	113	9.499	-94.178	123.637	1.00	32.27	B	C
	ATOM	2057	CG	LEU	113	8.480	-93.165	123.101	1.00	32.57	B	C
	ATOM	2058	CD1	LEU	113	7.983	-93.617	121.731	1.00	31.91	B	C
	ATOM	2059	CD2	LEU	113	7.325	-93.014	124.080	1.00	31.00	B	C
	ATOM	2060	C	LEU	113	11.380	-93.213	122.294	1.00	31.56	B	C
40	ATOM	2061	O	LEU	113	11.268	-92.799	121.138	1.00	30.78	B	O
	ATOM	2062	N	ILE	114	12.089	-92.586	123.227	1.00	30.06	B	N
	ATOM	2063	CA	ILE	114	12.808	-91.351	122.949	1.00	29.43	B	C
	ATOM	2064	CB	ILE	114	13.518	-90.822	124.221	1.00	28.14	B	C
	ATOM	2065	CG2	ILE	114	14.463	-89.686	123.870	1.00	27.33	B	C
45	ATOM	2066	CG1	ILE	114	12.472	-90.330	125.228	1.00	27.74	B	C
	ATOM	2067	CD1	ILE	114	13.058	-89.868	126.541	1.00	26.41	B	C
	ATOM	2068	C	ILE	114	13.837	-91.546	121.836	1.00	29.65	B	C
	ATOM	2069	O	ILE	114	13.866	-90.789	120.872	1.00	28.66	B	O
	ATOM	2070	N	ARG	115	14.672	-92.571	121.961	1.00	30.65	B	N
50	ATOM	2071	CA	ARG	115	15.686	-92.821	120.947	1.00	32.09	B	C
	ATOM	2072	CB	ARG	115	16.540	-94.037	121.319	1.00	34.79	B	C
	ATOM	2073	CG	ARG	115	17.947	-93.967	120.729	1.00	39.78	B	C
	ATOM	2074	CD	ARG	115	18.821	-95.166	121.077	1.00	43.64	B	C
	ATOM	2075	NE	ARG	115	18.482	-96.354	120.292	1.00	47.79	B	N
	ATOM	2076	CZ	ARG	115	17.535	-97.233	120.612	1.00	49.59	B	C
55	ATOM	2077	NH1	ARG	115	16.815	-97.074	121.713	1.00	51.59	B	N
	ATOM	2078	NH2	ARG	115	17.311	-98.281	119.832	1.00	50.36	B	N
	ATOM	2079	C	ARG	115	15.069	-93.016	119.562	1.00	30.91	B	C
	ATOM	2080	O	ARG	115	15.599	-92.516	118.571	1.00	31.00	B	O

-205-

	ATOM	2081	N	THR	116	13.952	-93.734	119.496	1.00	29.49	B	N
	ATOM	2082	CA	THR	116	13.263	-93.974	118.231	1.00	28.65	B	C
	ATOM	2083	CB	THR	116	12.058	-94.914	118.428	1.00	29.45	B	C
5	ATOM	2084	OG1	THR	116	12.514	-96.168	118.945	1.00	31.34	B	O
	ATOM	2085	CG2	THR	116	11.332	-95.147	117.112	1.00	29.40	B	C
	ATOM	2086	C	THR	116	12.757	-92.658	117.640	1.00	27.59	B	C
	ATOM	2087	O	THR	116	12.995	-92.359	116.469	1.00	27.35	B	O
	ATOM	2088	N	LEU	117	12.049	-91.882	118.455	1.00	25.67	B	N
10	ATOM	2089	CA	LEU	117	11.517	-90.594	118.019	1.00	24.51	B	C
	ATOM	2090	CB	LEU	117	10.691	-89.949	119.143	1.00	22.66	B	C
	ATOM	2091	CG	LEU	117	9.309	-90.544	119.437	1.00	23.35	B	C
	ATOM	2092	CD1	LEU	117	8.752	-89.953	120.731	1.00	22.38	B	C
	ATOM	2093	CD2	LEU	117	8.362	-90.261	118.270	1.00	22.82	B	C
15	ATOM	2094	C	LEU	117	12.647	-89.657	117.607	1.00	22.88	B	C
	ATOM	2095	O	LEU	117	12.566	-88.996	116.580	1.00	22.11	B	O
	ATOM	2096	N	LEU	118	13.698	-89.608	118.416	1.00	23.09	B	N
	ATOM	2097	CA	LEU	118	14.856	-88.755	118.152	1.00	23.66	B	C
	ATOM	2098	CB	LEU	118	15.879	-88.903	119.276	1.00	25.11	B	C
20	ATOM	2099	CG	LEU	118	16.702	-87.685	119.697	1.00	27.59	B	C
	ATOM	2100	CD1	LEU	118	18.037	-88.188	120.242	1.00	28.18	B	C
	ATOM	2101	CD2	LEU	118	16.932	-86.729	118.527	1.00	28.59	B	C
	ATOM	2102	C	LEU	118	15.520	-89.134	116.827	1.00	23.33	B	C
	ATOM	2103	O	LEU	118	15.921	-88.260	116.054	1.00	22.58	B	O
25	ATOM	2104	N	GLY	119	15.644	-90.441	116.585	1.00	22.04	B	N
	ATOM	2105	CA	GLY	119	16.255	-90.931	115.362	1.00	21.87	B	C
	ATOM	2106	C	GLY	119	15.491	-90.497	114.127	1.00	21.81	B	C
	ATOM	2107	O	GLY	119	16.072	-89.949	113.191	1.00	21.52	B	O
	ATOM	2108	N	ALA	120	14.185	-90.743	114.122	1.00	21.37	B	N
30	ATOM	2109	CA	ALA	120	13.331	-90.358	113.004	1.00	21.05	B	C
	ATOM	2110	CB	ALA	120	11.913	-90.885	113.233	1.00	20.81	B	C
	ATOM	2111	C	ALA	120	13.304	-88.829	112.833	1.00	21.40	B	C
	ATOM	2112	O	ALA	120	13.372	-88.314	111.716	1.00	20.48	B	O
	ATOM	2113	N	HIS	121	13.191	-88.110	113.945	1.00	22.14	B	N
35	ATOM	2114	CA	HIS	121	13.166	-86.649	113.914	1.00	22.47	B	C
	ATOM	2115	CB	HIS	121	12.936	-86.096	115.325	1.00	22.23	B	C
	ATOM	2116	CG	HIS	121	13.136	-84.619	115.433	1.00	24.18	B	C
	ATOM	2117	CD2	HIS	121	12.269	-83.589	115.284	1.00	23.87	B	C
	ATOM	2118	ND1	HIS	121	14.373	-84.050	115.657	1.00	24.73	B	N
40	ATOM	2119	CE1	HIS	121	14.258	-82.734	115.638	1.00	25.53	B	C
	ATOM	2120	NE2	HIS	121	12.992	-82.430	115.413	1.00	25.90	B	N
	ATOM	2121	C	HIS	121	14.469	-86.093	113.339	1.00	22.36	B	C
	ATOM	2122	O	HIS	121	14.452	-85.248	112.448	1.00	22.60	B	O
	ATOM	2123	N	THR	122	15.597	-86.574	113.849	1.00	21.59	B	N
45	ATOM	2124	CA	THR	122	16.900	-86.119	113.387	1.00	21.97	B	C
	ATOM	2125	CB	THR	122	18.038	-86.782	114.199	1.00	22.09	B	C
	ATOM	2126	OG1	THR	122	17.948	-86.364	115.561	1.00	24.17	B	O
	ATOM	2127	CG2	THR	122	19.397	-86.384	113.655	1.00	22.21	B	C
	ATOM	2128	C	THR	122	17.142	-86.400	111.907	1.00	21.55	B	C
50	ATOM	2129	O	THR	122	17.664	-85.549	111.188	1.00	20.90	B	O
	ATOM	2130	N	ARG	123	16.773	-87.595	111.455	1.00	21.32	B	N
	ATOM	2131	CA	ARG	123	16.990	-87.969	110.063	1.00	22.23	B	C
	ATOM	2132	CB	ARG	123	16.731	-89.472	109.852	1.00	21.90	B	C
	ATOM	2133	CG	ARG	123	17.899	-90.405	110.237	1.00	22.07	B	C
55	ATOM	2134	CD	ARG	123	17.662	-91.846	109.753	1.00	20.33	B	C
	ATOM	2135	NE	ARG	123	16.487	-92.450	110.380	1.00	21.86	B	N
	ATOM	2136	CZ	ARG	123	16.465	-92.979	111.601	1.00	21.57	B	C
	ATOM	2137	NH1	ARG	123	17.559	-93.002	112.352	1.00	21.63	B	N
	ATOM	2138	NH2	ARG	123	15.333	-93.467	112.086	1.00	20.21	B	N

-206-

	ATOM	2139	C	ARG	123	16.166	-87.193	109.043	1.00	22.64	B	C
	ATOM	2140	O	ARG	123	16.664	-86.867	107.971	1.00	23.15	B	O
	ATOM	2141	N	HIS	124	14.918	-86.877	109.370	1.00	22.90	B	N
5	ATOM	2142	CA	HIS	124	14.061	-86.204	108.398	1.00	23.53	B	C
	ATOM	2143	CB	HIS	124	12.841	-87.089	108.121	1.00	22.74	B	C
	ATOM	2144	CG	HIS	124	13.190	-88.501	107.763	1.00	23.34	B	C
	ATOM	2145	CD2	HIS	124	13.757	-89.023	106.650	1.00	22.54	B	C
	ATOM	2146	ND1	HIS	124	12.991	-89.562	108.624	1.00	22.99	B	N
10	ATOM	2147	CE1	HIS	124	13.421	-90.674	108.055	1.00	21.00	B	C
	ATOM	2148	NE2	HIS	124	13.891	-90.375	106.858	1.00	21.93	B	N
	ATOM	2149	C	HIS	124	13.588	-84.772	108.653	1.00	23.63	B	C
	ATOM	2150	O	HIS	124	13.238	-84.069	107.700	1.00	24.39	B	O
	ATOM	2151	N	MET	125	13.589	-84.322	109.905	1.00	22.90	B	N
15	ATOM	2152	CA	MET	125	13.097	-82.976	110.197	1.00	22.76	B	C
	ATOM	2153	CB	MET	125	11.817	-83.071	111.038	1.00	22.21	B	C
	ATOM	2154	CG	MET	125	10.710	-83.920	110.415	1.00	21.83	B	C
	ATOM	2155	SD	MET	125	9.120	-83.745	111.269	1.00	22.85	B	S
	ATOM	2156	CE	MET	125	9.499	-84.456	112.900	1.00	22.30	B	C
20	ATOM	2157	C	MET	125	14.065	-82.015	110.880	1.00	22.78	B	C
	ATOM	2158	O	MET	125	14.118	-80.833	110.530	1.00	22.22	B	O
	ATOM	2159	N	GLY	126	14.818	-82.527	111.852	1.00	22.55	B	N
	ATOM	2160	CA	GLY	126	15.758	-81.721	112.614	1.00	22.45	B	C
	ATOM	2161	C	GLY	126	16.466	-80.574	111.919	1.00	23.15	B	C
25	ATOM	2162	O	GLY	126	16.502	-79.458	112.438	1.00	23.04	B	O
	ATOM	2163	N	THR	127	17.047	-80.840	110.757	1.00	22.96	B	N
	ATOM	2164	CA	THR	127	17.756	-79.804	110.026	1.00	23.87	B	C
	ATOM	2165	CB	THR	127	19.261	-80.133	109.920	1.00	25.68	B	C
	ATOM	2166	OG1	THR	127	19.417	-81.510	109.569	1.00	27.25	B	O
30	ATOM	2167	CG2	THR	127	19.969	-79.868	111.242	1.00	26.03	B	C
	ATOM	2168	C	THR	127	17.203	-79.606	108.624	1.00	22.94	B	C
	ATOM	2169	O	THR	127	17.920	-79.166	107.728	1.00	22.72	B	O
	ATOM	2170	N	MET	128	15.927	-79.925	108.429	1.00	22.41	B	N
	ATOM	2171	CA	MET	128	15.320	-79.764	107.114	1.00	22.16	B	C
35	ATOM	2172	CB	MET	128	13.897	-80.330	107.101	1.00	21.38	B	C
	ATOM	2173	CG	MET	128	12.872	-79.579	107.943	1.00	20.15	B	C
	ATOM	2174	SD	MET	128	11.239	-80.338	107.749	1.00	20.67	B	S
	ATOM	2175	CE	MET	128	10.284	-79.362	108.917	1.00	22.56	B	C
	ATOM	2176	C	MET	128	15.305	-78.305	106.669	1.00	22.32	B	C
40	ATOM	2177	O	MET	128	15.261	-78.019	105.476	1.00	22.98	B	O
	ATOM	2178	N	PHE	129	15.363	-77.384	107.627	1.00	22.69	B	N
	ATOM	2179	CA	PHE	129	15.358	-75.957	107.311	1.00	24.34	B	C
	ATOM	2180	CB	PHE	129	15.281	-75.127	108.605	1.00	25.41	B	C
	ATOM	2181	CG	PHE	129	16.565	-75.092	109.396	1.00	28.48	B	C
45	ATOM	2182	CD1	PHE	129	17.588	-74.210	109.052	1.00	30.09	B	C
	ATOM	2183	CD2	PHE	129	16.749	-75.934	110.486	1.00	29.53	B	C
	ATOM	2184	CE1	PHE	129	18.775	-74.164	109.784	1.00	31.38	B	C
	ATOM	2185	CE2	PHE	129	17.928	-75.900	111.228	1.00	31.21	B	C
	ATOM	2186	CZ	PHE	129	18.945	-75.012	110.875	1.00	32.22	B	C
50	ATOM	2187	C	PHE	129	16.580	-75.540	106.485	1.00	24.09	B	C
	ATOM	2188	O	PHE	129	16.566	-74.501	105.821	1.00	23.81	B	O
	ATOM	2189	N	GLU	130	17.636	-76.346	106.522	1.00	24.21	B	N
	ATOM	2190	CA	GLU	130	18.843	-76.031	105.762	1.00	25.33	B	C
	ATOM	2191	CB	GLU	130	20.011	-76.906	106.222	1.00	27.28	B	C
55	ATOM	2192	CG	GLU	130	20.376	-76.718	107.685	1.00	31.35	B	C
	ATOM	2193	CD	GLU	130	21.694	-77.377	108.045	1.00	34.28	B	C
	ATOM	2194	OE1	GLU	130	22.057	-78.381	107.389	1.00	35.08	B	O
	ATOM	2195	OE2	GLU	130	22.360	-76.898	108.992	1.00	36.90	B	O
	ATOM	2196	C	GLU	130	18.647	-76.197	104.258	1.00	23.24	B	C

-207-

	ATOM	2197	O	GLU	130	19.439	-75.686	103.470	1.00	23.56	B	O
	ATOM	2198	N	GLN	131	17.601	-76.918	103.865	1.00	21.55	B	N
	ATOM	2199	CA	GLN	131	17.302	-77.125	102.453	1.00	20.76	B	C
5	ATOM	2200	CB	GLN	131	16.539	-78.442	102.240	1.00	21.85	B	C
	ATOM	2201	CG	GLN	131	17.320	-79.703	102.536	1.00	23.34	B	C
	ATOM	2202	CD	GLN	131	18.691	-79.696	101.882	1.00	26.07	B	C
	ATOM	2203	OE1	GLN	131	18.815	-79.538	100.664	1.00	26.66	B	O
	ATOM	2204	NE2	GLN	131	19.728	-79.862	102.692	1.00	26.55	B	N
10	ATOM	2205	C	GLN	131	16.462	-75.987	101.869	1.00	20.02	B	C
	ATOM	2206	O	GLN	131	16.346	-75.875	100.659	1.00	20.04	B	O
	ATOM	2207	N	PHE	132	15.880	-75.149	102.724	1.00	19.42	B	N
	ATOM	2208	CA	PHE	132	15.023	-74.048	102.269	1.00	19.05	B	C
	ATOM	2209	CB	PHE	132	14.612	-73.157	103.454	1.00	17.06	B	C
	ATOM	2210	CG	PHE	132	13.572	-73.779	104.384	1.00	16.44	B	C
15	ATOM	2211	CD1	PHE	132	13.055	-75.055	104.152	1.00	15.33	B	C
	ATOM	2212	CD2	PHE	132	13.117	-73.073	105.493	1.00	15.55	B	C
	ATOM	2213	CE1	PHE	132	12.099	-75.620	105.018	1.00	15.93	B	C
	ATOM	2214	CE2	PHE	132	12.157	-73.626	106.368	1.00	15.23	B	C
20	ATOM	2215	CZ	PHE	132	11.651	-74.895	106.132	1.00	15.15	B	C
	ATOM	2216	C	PHE	132	15.650	-73.182	101.170	1.00	19.75	B	C
	ATOM	2217	O	PHE	132	14.957	-72.736	100.254	1.00	19.12	B	O
	ATOM	2218	N	VAL	133	16.955	-72.946	101.266	1.00	20.25	B	N
	ATOM	2219	CA	VAL	133	17.675	-72.139	100.287	1.00	21.53	B	C
25	ATOM	2220	CB	VAL	133	19.135	-71.915	100.737	1.00	22.78	B	C
	ATOM	2221	CG1	VAL	133	19.901	-73.236	100.711	1.00	21.70	B	C
	ATOM	2222	CG2	VAL	133	19.799	-70.870	99.850	1.00	23.73	B	C
	ATOM	2223	C	VAL	133	17.673	-72.750	98.877	1.00	22.37	B	C
	ATOM	2224	O	VAL	133	17.955	-72.058	97.895	1.00	21.91	B	O
30	ATOM	2225	N	GLN	134	17.344	-74.036	98.780	1.00	22.29	B	N
	ATOM	2226	CA	GLN	134	17.294	-74.725	97.496	1.00	23.37	B	C
	ATOM	2227	CB	GLN	134	17.558	-76.229	97.680	1.00	22.92	B	C
	ATOM	2228	CG	GLN	134	18.860	-76.621	98.407	1.00	23.40	B	C
	ATOM	2229	CD	GLN	134	20.154	-76.250	97.659	1.00	23.05	B	C
35	ATOM	2230	OE1	GLN	134	21.237	-76.701	98.020	1.00	25.27	B	O
	ATOM	2231	NE2	GLN	134	20.042	-75.430	96.639	1.00	22.55	B	N
	ATOM	2232	C	GLN	134	15.954	-74.548	96.768	1.00	24.55	B	C
	ATOM	2233	O	GLN	134	15.771	-75.081	95.678	1.00	24.39	B	O
	ATOM	2234	N	PHE	135	15.022	-73.804	97.361	1.00	24.64	B	N
40	ATOM	2235	CA	PHE	135	13.710	-73.595	96.750	1.00	25.44	B	C
	ATOM	2236	CB	PHE	135	12.626	-74.065	97.722	1.00	24.79	B	C
	ATOM	2237	CG	PHE	135	12.706	-75.534	98.039	1.00	23.89	B	C
	ATOM	2238	CD1	PHE	135	12.206	-76.478	97.146	1.00	24.40	B	C
	ATOM	2239	CD2	PHE	135	13.335	-75.977	99.198	1.00	24.10	B	C
45	ATOM	2240	CE1	PHE	135	12.331	-77.848	97.397	1.00	24.28	B	C
	ATOM	2241	CE2	PHE	135	13.470	-77.349	99.466	1.00	24.09	B	C
	ATOM	2242	CZ	PHE	135	12.966	-78.286	98.560	1.00	24.17	B	C
	ATOM	2243	C	PHE	135	13.500	-72.130	96.358	1.00	27.05	B	C
	ATOM	2244	O	PHE	135	12.508	-71.501	96.739	1.00	27.09	B	O
50	ATOM	2245	N	ARG	136	14.444	-71.622	95.566	1.00	27.76	B	N
	ATOM	2246	CA	ARG	136	14.486	-70.241	95.098	1.00	28.77	B	C
	ATOM	2247	CB	ARG	136	14.046	-70.118	93.626	1.00	30.48	B	C
	ATOM	2248	CG	ARG	136	12.754	-70.801	93.245	1.00	34.79	B	C
	ATOM	2249	CD	ARG	136	13.002	-72.190	92.685	1.00	36.21	B	C
55	ATOM	2250	NE	ARG	136	11.998	-73.127	93.184	1.00	39.78	B	N
	ATOM	2251	CZ	ARG	136	12.120	-74.448	93.158	1.00	40.31	B	C
	ATOM	2252	NH1	ARG	136	13.214	-75.011	92.649	1.00	41.22	B	N
	ATOM	2253	NH2	ARG	136	11.152	-75.207	93.654	1.00	40.63	B	N
	ATOM	2254	C	ARG	136	13.765	-69.204	95.951	1.00	28.40	B	C

-208-

	ATOM	2255	O	ARG	136	12.679	-68.725	95.618	1.00	27.33	B	O
	ATOM	2256	N	PRO	137	14.379	-68.850	97.085	1.00	28.01	B	N
	ATOM	2257	CD	PRO	137	15.580	-69.475	97.667	1.00	27.43	B	C
5	ATOM	2258	CA	PRO	137	13.821	-67.860	97.999	1.00	27.65	B	C
	ATOM	2259	CB	PRO	137	14.586	-68.120	99.286	1.00	27.04	B	C
	ATOM	2260	CG	PRO	137	15.924	-68.518	98.778	1.00	27.95	B	C
	ATOM	2261	C	PRO	137	14.108	-66.467	97.451	1.00	27.46	B	C
	ATOM	2262	O	PRO	137	15.212	-66.190	96.981	1.00	27.51	B	O
10	ATOM	2263	N	PRO	138	13.110	-65.578	97.479	1.00	26.95	B	N
	ATOM	2264	CD	PRO	138	11.696	-65.734	97.852	1.00	26.96	B	C
	ATOM	2265	CA	PRO	138	13.372	-64.234	96.968	1.00	26.24	B	C
	ATOM	2266	CB	PRO	138	12.051	-63.496	97.228	1.00	26.54	B	C
	ATOM	2267	CG	PRO	138	11.350	-64.341	98.273	1.00	27.40	B	C
15	ATOM	2268	C	PRO	138	14.573	-63.608	97.679	1.00	25.08	B	C
	ATOM	2269	O	PRO	138	14.928	-63.992	98.799	1.00	23.40	B	O
	ATOM	2270	N	ALA	139	15.194	-62.642	97.014	1.00	24.45	B	N
	ATOM	2271	CA	ALA	139	16.377	-61.959	97.529	1.00	24.74	B	C
	ATOM	2272	CB	ALA	139	16.852	-60.925	96.503	1.00	25.14	B	C
20	ATOM	2273	C	ALA	139	16.283	-61.300	98.905	1.00	24.49	B	C
	ATOM	2274	O	ALA	139	17.268	-61.293	99.651	1.00	24.23	B	O
	ATOM	2275	N	HIS	140	15.120	-60.749	99.252	1.00	24.55	B	N
	ATOM	2276	CA	HIS	140	14.979	-60.066	100.543	1.00	24.29	B	C
	ATOM	2277	CB	HIS	140	13.677	-59.245	100.587	1.00	23.87	B	C
25	ATOM	2278	CG	HIS	140	12.440	-60.056	100.826	1.00	23.38	B	C
	ATOM	2279	CD2	HIS	140	11.696	-60.232	101.944	1.00	23.33	B	C
	ATOM	2280	ND1	HIS	140	11.817	-60.783	99.833	1.00	23.88	B	N
	ATOM	2281	CE1	HIS	140	10.743	-61.371	100.328	1.00	24.02	B	C
	ATOM	2282	NE2	HIS	140	10.647	-61.054	101.608	1.00	24.40	B	N
30	ATOM	2283	C	HIS	140	15.080	-60.951	101.790	1.00	24.34	B	C
	ATOM	2284	O	HIS	140	15.223	-60.439	102.901	1.00	24.05	B	O
	ATOM	2285	N	LEU	141	15.010	-62.265	101.605	1.00	24.45	B	N
	ATOM	2286	CA	LEU	141	15.117	-63.216	102.714	1.00	25.64	B	C
	ATOM	2287	CB	LEU	141	14.436	-64.544	102.352	1.00	24.52	B	C
35	ATOM	2288	CG	LEU	141	12.951	-64.562	101.981	1.00	25.14	B	C
	ATOM	2289	CD1	LEU	141	12.529	-65.992	101.647	1.00	23.52	B	C
	ATOM	2290	CD2	LEU	141	12.118	-64.006	103.143	1.00	23.73	B	C
	ATOM	2291	C	LEU	141	16.577	-63.512	103.056	1.00	26.62	B	C
	ATOM	2292	O	LEU	141	16.886	-64.005	104.138	1.00	26.38	B	O
40	ATOM	2293	N	PHE	142	17.476	-63.213	102.130	1.00	28.49	B	N
	ATOM	2294	CA	PHE	142	18.888	-63.495	102.331	1.00	31.82	B	C
	ATOM	2295	CB	PHE	142	19.611	-63.519	100.985	1.00	29.28	B	C
	ATOM	2296	CG	PHE	142	19.392	-64.779	100.212	1.00	27.30	B	C
	ATOM	2297	CD1	PHE	142	20.232	-65.873	100.393	1.00	25.11	B	C
	ATOM	2298	CD2	PHE	142	18.323	-64.890	99.331	1.00	26.50	B	C
45	ATOM	2299	CE1	PHE	142	20.010	-67.056	99.706	1.00	25.73	B	C
	ATOM	2300	CE2	PHE	142	18.093	-66.074	98.639	1.00	26.27	B	C
	ATOM	2301	CZ	PHE	142	18.937	-67.159	98.826	1.00	25.25	B	C
	ATOM	2302	C	PHE	142	19.648	-62.591	103.275	1.00	35.28	B	C
50	ATOM	2303	O	PHE	142	19.462	-61.377	103.281	1.00	35.57	B	O
	ATOM	2304	N	ILE	143	20.503	-63.228	104.071	1.00	39.02	B	N
	ATOM	2305	CA	ILE	143	21.385	-62.575	105.028	1.00	42.74	B	C
	ATOM	2306	CB	ILE	143	22.843	-62.584	104.472	1.00	42.59	B	C
	ATOM	2307	CG2	ILE	143	23.827	-62.089	105.529	1.00	42.50	B	C
	ATOM	2308	CG1	ILE	143	23.209	-64.007	104.032	1.00	42.81	B	C
55	ATOM	2309	CD1	ILE	143	24.580	-64.142	103.438	1.00	43.32	B	C
	ATOM	2310	C	ILE	143	20.970	-61.147	105.388	1.00	45.22	B	C
	ATOM	2311	O	ILE	143	20.209	-60.940	106.333	1.00	46.12	B	O
	ATOM	2312	N	HIS	144	21.462	-60.165	104.636	1.00	48.10	B	N

-209-

	ATOM	2313	CA	HIS	144	21.138	-58.766	104.905	1.00	50.43	B	C
	ATOM	2314	CB	HIS	144	22.347	-58.077	105.549	1.00	51.71	B	C
	ATOM	2315	CG	HIS	144	22.639	-58.553	106.941	1.00	53.18	B	C
5	ATOM	2316	CD2	HIS	144	21.840	-59.129	107.873	1.00	53.68	B	C
	ATOM	2317	ND1	HIS	144	23.885	-58.447	107.520	1.00	53.87	B	N
	ATOM	2318	CE1	HIS	144	23.843	-58.939	108.747	1.00	53.89	B	C
	ATOM	2319	NE2	HIS	144	22.613	-59.360	108.985	1.00	53.40	B	N
	ATOM	2320	C	HIS	144	20.688	-58.010	103.655	1.00	50.90	B	C
10	ATOM	2321	O	HIS	144	21.479	-57.322	103.006	1.00	51.65	B	O
	ATOM	2322	N	HIS	145	19.403	-58.149	103.339	1.00	51.36	B	N
	ATOM	2323	CA	HIS	145	18.778	-57.503	102.183	1.00	51.48	B	C
	ATOM	2324	CB	HIS	145	18.251	-58.577	101.223	1.00	52.46	B	C
	ATOM	2325	CG	HIS	145	18.066	-58.105	99.812	1.00	53.73	B	C
15	ATOM	2326	CD2	HIS	145	16.958	-57.714	99.140	1.00	54.04	B	C
	ATOM	2327	ND1	HIS	145	19.109	-58.015	98.915	1.00	54.94	B	N
	ATOM	2328	CE1	HIS	145	18.651	-57.592	97.750	1.00	54.82	B	C
	ATOM	2329	NE2	HIS	145	17.348	-57.401	97.859	1.00	54.54	B	N
	ATOM	2330	C	HIS	145	17.610	-56.629	102.673	1.00	50.58	B	C
20	ATOM	2331	O	HIS	145	16.980	-56.929	103.691	1.00	50.62	B	O
	ATOM	2332	N	GLN	146	17.325	-55.552	101.950	1.00	49.68	B	N
	ATOM	2333	CA	GLN	146	16.227	-54.650	102.303	1.00	48.58	B	C
	ATOM	2334	CB	GLN	146	16.264	-53.426	101.373	1.00	50.29	B	C
	ATOM	2335	CG	GLN	146	15.242	-52.329	101.656	1.00	52.37	B	C
25	ATOM	2336	CD	GLN	146	14.090	-52.316	100.661	1.00	53.97	B	C
	ATOM	2337	OE1	GLN	146	14.299	-52.395	99.446	1.00	55.36	B	O
	ATOM	2338	NE2	GLN	146	12.867	-52.216	101.172	1.00	53.39	B	N
	ATOM	2339	C	GLN	146	14.902	-55.412	102.152	1.00	46.43	B	C
	ATOM	2340	O	GLN	146	14.772	-56.250	101.259	1.00	47.01	B	O
30	ATOM	2341	N	PRO	147	13.906	-55.140	103.024	1.00	43.87	B	N
	ATOM	2342	CD	PRO	147	13.896	-54.126	104.094	1.00	42.94	B	C
	ATOM	2343	CA	PRO	147	12.604	-55.823	102.952	1.00	40.85	B	C
	ATOM	2344	CB	PRO	147	11.805	-55.171	104.081	1.00	41.31	B	C
	ATOM	2345	CG	PRO	147	12.427	-53.812	104.211	1.00	42.30	B	C
35	ATOM	2346	C	PRO	147	11.911	-55.697	101.594	1.00	37.44	B	C
	ATOM	2347	O	PRO	147	12.368	-54.956	100.733	1.00	36.62	B	O
	ATOM	2348	N	LEU	148	10.812	-56.428	101.408	1.00	34.45	B	N
	ATOM	2349	CA	LEU	148	10.076	-56.402	100.143	1.00	31.79	B	C
	ATOM	2350	CB	LEU	148	8.912	-57.397	100.162	1.00	30.82	B	C
40	ATOM	2351	CG	LEU	148	8.883	-58.528	99.124	1.00	31.47	B	C
	ATOM	2352	CD1	LEU	148	7.437	-58.918	98.878	1.00	30.58	B	C
	ATOM	2353	CD2	LEU	148	9.531	-58.102	97.817	1.00	30.15	B	C
	ATOM	2354	C	LEU	148	9.521	-55.018	99.849	1.00	29.43	B	C
	ATOM	2355	O	LEU	148	8.779	-54.456	100.653	1.00	28.77	B	O
45	ATOM	2356	N	PRO	149	9.871	-54.448	98.690	1.00	27.64	B	N
	ATOM	2357	CD	PRO	149	10.846	-54.900	97.686	1.00	27.10	B	C
	ATOM	2358	CA	PRO	149	9.358	-53.114	98.361	1.00	26.65	B	C
	ATOM	2359	CB	PRO	149	9.986	-52.829	96.998	1.00	26.71	B	C
	ATOM	2360	CG	PRO	149	11.296	-53.591	97.075	1.00	26.43	B	C
50	ATOM	2361	C	PRO	149	7.833	-53.103	98.311	1.00	25.49	B	C
	ATOM	2362	O	PRO	149	7.201	-54.132	98.090	1.00	25.29	B	O
	ATOM	2363	N	THR	150	7.248	-51.932	98.516	1.00	24.33	B	N
	ATOM	2364	CA	THR	150	5.799	-51.782	98.494	1.00	23.46	B	C
	ATOM	2365	CB	THR	150	5.417	-50.287	98.643	1.00	23.36	B	C
	ATOM	2366	OG1	THR	150	5.760	-49.841	99.964	1.00	21.71	B	O
55	ATOM	2367	CG2	THR	150	3.934	-50.077	98.395	1.00	22.73	B	C
	ATOM	2368	C	THR	150	5.120	-52.357	97.244	1.00	23.83	B	C
	ATOM	2369	O	THR	150	4.111	-53.056	97.346	1.00	24.37	B	O
	ATOM	2370	N	LEU	151	5.671	-52.075	96.071	1.00	23.39	B	N

-210-

5	ATOM	2371	CA	LEU	151	5.086	-52.549	94.818	1.00	24.18	B	C
	ATOM	2372	CB	LEU	151	5.174	-51.435	93.764	1.00	23.98	B	C
	ATOM	2373	CG	LEU	151	3.943	-50.542	93.516	1.00	26.19	B	C
	ATOM	2374	CD1	LEU	151	3.125	-50.352	94.783	1.00	25.29	B	C
	ATOM	2375	CD2	LEU	151	4.406	-49.199	92.956	1.00	25.33	B	C
10	ATOM	2376	C	LEU	151	5.692	-53.843	94.256	1.00	24.80	B	C
	ATOM	2377	O	LEU	151	5.289	-54.307	93.188	1.00	24.09	B	O
	ATOM	2378	N	ALA	152	6.651	-54.433	94.965	1.00	25.14	B	N
	ATOM	2379	CA	ALA	152	7.269	-55.666	94.485	1.00	25.42	B	C
	ATOM	2380	CB	ALA	152	8.449	-56.032	95.357	1.00	25.27	B	C
15	ATOM	2381	C	ALA	152	6.255	-56.800	94.483	1.00	25.45	B	C
	ATOM	2382	O	ALA	152	5.516	-56.990	95.447	1.00	26.33	B	O
	ATOM	2383	N	PRO	153	6.182	-57.558	93.385	1.00	25.59	B	N
	ATOM	2384	CD	PRO	153	6.844	-57.411	92.078	1.00	26.03	B	C
	ATOM	2385	CA	PRO	153	5.214	-58.658	93.373	1.00	25.15	B	C
20	ATOM	2386	CB	PRO	153	5.337	-59.222	91.953	1.00	25.93	B	C
	ATOM	2387	CG	PRO	153	6.712	-58.795	91.514	1.00	27.37	B	C
	ATOM	2388	C	PRO	153	5.538	-59.683	94.457	1.00	24.29	B	C
	ATOM	2389	O	PRO	153	6.705	-59.912	94.776	1.00	23.77	B	O
	ATOM	2390	N	VAL	154	4.502	-60.283	95.031	1.00	23.14	B	N
25	ATOM	2391	CA	VAL	154	4.689	-61.269	96.090	1.00	23.20	B	C
	ATOM	2392	CB	VAL	154	3.612	-61.118	97.205	1.00	23.14	B	C
	ATOM	2393	CG1	VAL	154	3.638	-59.705	97.761	1.00	24.25	B	C
	ATOM	2394	CG2	VAL	154	2.233	-61.440	96.656	1.00	22.99	B	C
	ATOM	2395	C	VAL	154	4.669	-62.710	95.589	1.00	22.02	B	C
30	ATOM	2396	O	VAL	154	4.882	-63.631	96.364	1.00	21.64	B	O
	ATOM	2397	N	LEU	155	4.413	-62.901	94.298	1.00	21.95	B	N
	ATOM	2398	CA	LEU	155	4.374	-64.244	93.711	1.00	21.77	B	C
	ATOM	2399	CB	LEU	155	4.170	-64.164	92.191	1.00	21.08	B	C
	ATOM	2400	CG	LEU	155	4.166	-65.490	91.410	1.00	22.05	B	C
35	ATOM	2401	CD1	LEU	155	3.033	-66.385	91.892	1.00	20.48	B	C
	ATOM	2402	CD2	LEU	155	4.017	-65.204	89.905	1.00	22.31	B	C
	ATOM	2403	C	LEU	155	5.622	-65.083	94.030	1.00	20.95	B	C
	ATOM	2404	O	LEU	155	5.496	-66.258	94.373	1.00	21.26	B	O
	ATOM	2405	N	PRO	156	6.838	-64.505	93.908	1.00	20.25	B	N
40	ATOM	2406	CD	PRO	156	7.210	-63.205	93.313	1.00	20.55	B	C
	ATOM	2407	CA	PRO	156	8.040	-65.294	94.218	1.00	20.02	B	C
	ATOM	2408	CB	PRO	156	9.178	-64.316	93.942	1.00	19.60	B	C
	ATOM	2409	CG	PRO	156	8.627	-63.462	92.821	1.00	19.34	B	C
	ATOM	2410	C	PRO	156	8.043	-65.793	95.675	1.00	20.44	B	C
45	ATOM	2411	O	PRO	156	8.401	-66.943	95.948	1.00	18.86	B	O
	ATOM	2412	N	LEU	157	7.646	-64.922	96.603	1.00	18.95	B	N
	ATOM	2413	CA	LEU	157	7.584	-65.298	98.012	1.00	18.72	B	C
	ATOM	2414	CB	LEU	157	7.243	-64.086	98.886	1.00	18.06	B	C
	ATOM	2415	CG	LEU	157	7.139	-64.367	100.390	1.00	18.20	B	C
50	ATOM	2416	CD1	LEU	157	8.459	-64.931	100.910	1.00	18.30	B	C
	ATOM	2417	CD2	LEU	157	6.800	-63.078	101.133	1.00	18.86	B	C
	ATOM	2418	C	LEU	157	6.524	-66.376	98.210	1.00	18.16	B	C
	ATOM	2419	O	LEU	157	6.762	-67.369	98.892	1.00	17.47	B	O
	ATOM	2420	N	VAL	158	5.353	-66.174	97.612	1.00	17.84	B	N
55	ATOM	2421	CA	VAL	158	4.254	-67.132	97.713	1.00	18.75	B	C
	ATOM	2422	CB	VAL	158	3.016	-66.637	96.928	1.00	19.19	B	C
	ATOM	2423	CG1	VAL	158	1.971	-67.746	96.840	1.00	18.53	B	C
	ATOM	2424	CG2	VAL	158	2.431	-65.397	97.610	1.00	19.01	B	C
	ATOM	2425	C	VAL	158	4.656	-68.504	97.167	1.00	19.26	B	C
	ATOM	2426	O	VAL	158	4.372	-69.539	97.773	1.00	17.72	B	O
	ATOM	2427	N	THR	159	5.306	-68.504	96.009	1.00	19.18	B	N
	ATOM	2428	CA	THR	159	5.749	-69.742	95.382	1.00	20.12	B	C

-211-

	ATOM	2429	CB	THR	159	6.359	-69.464	94.005	1.00	20.73	B	C
	ATOM	2430	OG1	THR	159	5.429	-68.696	93.233	1.00	21.98	B	O
	ATOM	2431	CG2	THR	159	6.670	-70.780	93.277	1.00	20.98	B	C
5	ATOM	2432	C	THR	159	6.786	-70.418	96.270	1.00	19.12	B	C
	ATOM	2433	O	THR	159	6.757	-71.631	96.447	1.00	19.81	B	O
	ATOM	2434	N	HIS	160	7.695	-69.624	96.827	1.00	18.60	B	N
	ATOM	2435	CA	HIS	160	8.725	-70.143	97.722	1.00	19.62	B	C
	ATOM	2436	CB	HIS	160	9.628	-69.004	98.201	1.00	19.12	B	C
10	ATOM	2437	CG	HIS	160	10.583	-69.405	99.283	1.00	20.97	B	C
	ATOM	2438	CD2	HIS	160	10.739	-68.946	100.548	1.00	19.99	B	C
	ATOM	2439	ND1	HIS	160	11.547	-70.374	99.106	1.00	21.00	B	N
	ATOM	2440	CE1	HIS	160	12.258	-70.492	100.214	1.00	20.06	B	C
	ATOM	2441	NE2	HIS	160	11.787	-69.637	101.103	1.00	18.80	B	N
15	ATOM	2442	C	HIS	160	8.069	-70.835	98.922	1.00	18.85	B	C
	ATOM	2443	O	HIS	160	8.465	-71.934	99.309	1.00	19.48	B	O
	ATOM	2444	N	PHE	161	7.065	-70.192	99.510	1.00	18.30	B	N
	ATOM	2445	CA	PHE	161	6.362	-70.783	100.644	1.00	17.81	B	C
	ATOM	2446	CB	PHE	161	5.333	-69.799	101.218	1.00	17.09	B	C
20	ATOM	2447	CG	PHE	161	5.924	-68.773	102.167	1.00	18.77	B	C
	ATOM	2448	CD1	PHE	161	7.253	-68.861	102.576	1.00	18.08	B	C
	ATOM	2449	CD2	PHE	161	5.137	-67.743	102.675	1.00	18.45	B	C
	ATOM	2450	CE1	PHE	161	7.788	-67.943	103.478	1.00	19.86	B	C
	ATOM	2451	CE2	PHE	161	5.658	-66.818	103.577	1.00	19.78	B	C
25	ATOM	2452	CZ	PHE	161	6.992	-66.918	103.981	1.00	20.06	B	C
	ATOM	2453	C	PHE	161	5.675	-72.081	100.227	1.00	17.47	B	C
	ATOM	2454	O	PHE	161	5.721	-73.075	100.953	1.00	16.02	B	O
	ATOM	2455	N	ALA	162	5.039	-72.082	99.058	1.00	16.64	B	N
	ATOM	2456	CA	ALA	162	4.361	-73.286	98.588	1.00	17.85	B	C
30	ATOM	2457	CB	ALA	162	3.712	-73.034	97.224	1.00	17.30	B	C
	ATOM	2458	C	ALA	162	5.352	-74.447	98.487	1.00	18.28	B	C
	ATOM	2459	O	ALA	162	5.055	-75.563	98.899	1.00	17.59	B	O
	ATOM	2460	N	ASP	163	6.530	-74.166	97.935	1.00	18.81	B	N
	ATOM	2461	CA	ASP	163	7.569	-75.170	97.763	1.00	20.29	B	C
35	ATOM	2462	CB	ASP	163	8.650	-74.624	96.834	1.00	21.76	B	C
	ATOM	2463	CG	ASP	163	8.147	-74.448	95.414	1.00	22.93	B	C
	ATOM	2464	OD1	ASP	163	8.816	-73.763	94.621	1.00	25.09	B	O
	ATOM	2465	OD2	ASP	163	7.080	-75.005	95.093	1.00	23.14	B	O
	ATOM	2466	C	ASP	163	8.183	-75.671	99.072	1.00	20.12	B	C
40	ATOM	2467	O	ASP	163	8.307	-76.873	99.258	1.00	18.59	B	O
	ATOM	2468	N	ILE	164	8.564	-74.780	99.986	1.00	19.96	B	N
	ATOM	2469	CA	ILE	164	9.117	-75.286	101.240	1.00	20.35	B	C
	ATOM	2470	CB	ILE	164	9.877	-74.193	102.071	1.00	20.04	B	C
	ATOM	2471	CG2	ILE	164	11.003	-73.596	101.224	1.00	19.12	B	C
45	ATOM	2472	CG1	ILE	164	8.934	-73.093	102.555	1.00	20.01	B	C
	ATOM	2473	CD1	ILE	164	9.619	-72.108	103.497	1.00	18.11	B	C
	ATOM	2474	C	ILE	164	8.014	-75.950	102.076	1.00	20.60	B	C
	ATOM	2475	O	ILE	164	8.287	-76.890	102.819	1.00	20.54	B	O
	ATOM	2476	N	ASN	165	6.766	-75.496	101.939	1.00	19.91	B	N
50	ATOM	2477	CA	ASN	165	5.664	-76.123	102.673	1.00	19.83	B	C
	ATOM	2478	CB	ASN	165	4.341	-75.370	102.464	1.00	18.46	B	C
	ATOM	2479	CG	ASN	165	4.268	-74.061	103.244	1.00	19.03	B	C
	ATOM	2480	OD1	ASN	165	5.070	-73.812	104.145	1.00	17.31	B	O
	ATOM	2481	ND2	ASN	165	3.290	-73.221	102.900	1.00	17.09	B	N
55	ATOM	2482	C	ASN	165	5.497	-77.565	102.174	1.00	20.04	B	C
	ATOM	2483	O	ASN	165	5.334	-78.500	102.960	1.00	19.45	B	O
	ATOM	2484	N	THR	166	5.525	-77.741	100.859	1.00	20.25	B	N
	ATOM	2485	CA	THR	166	5.379	-79.071	100.279	1.00	20.86	B	C
	ATOM	2486	CB	THR	166	5.359	-78.981	98.741	1.00	21.41	B	C

-212-

5	ATOM	2487	OG1	THR	166	4.211	-78.224	98.341	1.00	22.00	B	O
	ATOM	2488	CG2	THR	166	5.293	-80.368	98.104	1.00	20.43	B	C
	ATOM	2489	C	THR	166	6.537	-79.947	100.759	1.00	20.47	B	C
	ATOM	2490	O	THR	166	6.338	-81.079	101.198	1.00	19.94	B	O
	ATOM	2491	N	PHE	167	7.745	-79.403	100.682	1.00	19.96	B	N
10	ATOM	2492	CA	PHE	167	8.944	-80.099	101.133	1.00	20.53	B	C
	ATOM	2493	CB	PHE	167	10.153	-79.166	100.994	1.00	20.58	B	C
	ATOM	2494	CG	PHE	167	11.373	-79.620	101.752	1.00	21.61	B	C
	ATOM	2495	CD1	PHE	167	12.098	-80.739	101.338	1.00	21.76	B	C
	ATOM	2496	CD2	PHE	167	11.812	-78.909	102.868	1.00	20.70	B	C
15	ATOM	2497	CE1	PHE	167	13.254	-81.145	102.025	1.00	22.38	B	C
	ATOM	2498	CE2	PHE	167	12.959	-79.303	103.563	1.00	22.67	B	C
	ATOM	2499	CZ	PHE	167	13.685	-80.426	103.137	1.00	22.67	B	C
	ATOM	2500	C	PHE	167	8.790	-80.557	102.592	1.00	20.25	B	C
	ATOM	2501	O	PHE	167	9.011	-81.730	102.904	1.00	20.74	B	O
20	ATOM	2502	N	MET	168	8.403	-79.640	103.479	1.00	18.80	B	N
	ATOM	2503	CA	MET	168	8.235	-79.971	104.897	1.00	18.84	B	C
	ATOM	2504	CB	MET	168	7.858	-78.722	105.712	1.00	17.54	B	C
	ATOM	2505	CG	MET	168	9.004	-77.727	105.904	1.00	16.54	B	C
	ATOM	2506	SD	MET	168	8.609	-76.401	107.082	1.00	16.62	B	S
25	ATOM	2507	CE	MET	168	7.812	-75.178	106.019	1.00	15.56	B	C
	ATOM	2508	C	MET	168	7.215	-81.078	105.163	1.00	18.68	B	C
	ATOM	2509	O	MET	168	7.461	-81.969	105.970	1.00	17.64	B	O
	ATOM	2510	N	VAL	169	6.065	-81.024	104.503	1.00	19.45	B	N
	ATOM	2511	CA	VAL	169	5.057	-82.064	104.702	1.00	20.76	B	C
30	ATOM	2512	CB	VAL	169	3.770	-81.768	103.889	1.00	21.33	B	C
	ATOM	2513	CG1	VAL	169	2.833	-82.969	103.936	1.00	20.85	B	C
	ATOM	2514	CG2	VAL	169	3.072	-80.531	104.458	1.00	21.08	B	C
	ATOM	2515	C	VAL	169	5.642	-83.414	104.275	1.00	21.26	B	C
	ATOM	2516	O	VAL	169	5.475	-84.420	104.965	1.00	20.54	B	O
35	ATOM	2517	N	LEU	170	6.337	-83.435	103.139	1.00	21.18	B	N
	ATOM	2518	CA	LEU	170	6.959	-84.670	102.659	1.00	21.80	B	C
	ATOM	2519	CB	LEU	170	7.695	-84.421	101.338	1.00	22.86	B	C
	ATOM	2520	CG	LEU	170	6.802	-84.091	100.139	1.00	24.31	B	C
	ATOM	2521	CD1	LEU	170	7.655	-83.710	98.941	1.00	24.24	B	C
40	ATOM	2522	CD2	LEU	170	5.928	-85.300	99.818	1.00	24.97	B	C
	ATOM	2523	C	LEU	170	7.942	-85.212	103.702	1.00	21.40	B	C
	ATOM	2524	O	LEU	170	8.051	-86.426	103.891	1.00	20.50	B	O
	ATOM	2525	N	GLN	171	8.660	-84.312	104.371	1.00	20.25	B	N
	ATOM	2526	CA	GLN	171	9.609	-84.721	105.402	1.00	20.37	B	C
45	ATOM	2527	CB	GLN	171	10.510	-83.544	105.808	1.00	18.76	B	C
	ATOM	2528	CG	GLN	171	11.490	-83.112	104.719	1.00	17.74	B	C
	ATOM	2529	CD	GLN	171	12.377	-84.259	104.254	1.00	18.92	B	C
	ATOM	2530	OE1	GLN	171	13.124	-84.841	105.034	1.00	20.91	B	O
	ATOM	2531	NE2	GLN	171	12.290	-84.590	102.987	1.00	17.61	B	N
50	ATOM	2532	C	GLN	171	8.879	-85.276	106.626	1.00	20.12	B	C
	ATOM	2533	O	GLN	171	9.344	-86.229	107.249	1.00	19.85	B	O
	ATOM	2534	N	VAL	172	7.740	-84.677	106.971	1.00	20.71	B	N
	ATOM	2535	CA	VAL	172	6.944	-85.137	108.112	1.00	21.73	B	C
	ATOM	2536	CB	VAL	172	5.733	-84.207	108.363	1.00	22.96	B	C
55	ATOM	2537	CG1	VAL	172	4.789	-84.833	109.384	1.00	22.67	B	C
	ATOM	2538	CG2	VAL	172	6.222	-82.851	108.874	1.00	22.87	B	C
	ATOM	2539	C	VAL	172	6.442	-86.561	107.853	1.00	21.64	B	C
	ATOM	2540	O	VAL	172	6.419	-87.408	108.755	1.00	20.64	B	O
	ATOM	2541	N	ILE	173	6.044	-86.815	106.612	1.00	21.03	B	N
	ATOM	2542	CA	ILE	173	5.579	-88.132	106.219	1.00	21.75	B	C
	ATOM	2543	CB	ILE	173	5.130	-88.135	104.725	1.00	21.85	B	C
	ATOM	2544	CG2	ILE	173	4.791	-89.563	104.271	1.00	22.44	B	C

-213-

	ATOM	2545	CG1	ILE	173	3.908	-87.222	104.561	1.00	21.48	B	C
	ATOM	2546	CD1	ILE	173	3.360	-87.129	103.143	1.00	20.80	B	C
	ATOM	2547	C	ILE	173	6.725	-89.126	106.449	1.00	21.99	B	C
5	ATOM	2548	O	ILE	173	6.512	-90.212	106.986	1.00	20.98	B	O
	ATOM	2549	N	LYS	174	7.942	-88.742	106.057	1.00	22.27	B	N
	ATOM	2550	CA	LYS	174	9.117	-89.596	106.252	1.00	22.72	B	C
	ATOM	2551	CB	LYS	174	10.365	-88.925	105.671	1.00	23.87	B	C
	ATOM	2552	CG	LYS	174	10.571	-89.108	104.171	1.00	27.23	B	C
10	ATOM	2553	CD	LYS	174	11.763	-88.274	103.704	1.00	29.56	B	C
	ATOM	2554	CE	LYS	174	12.282	-88.701	102.342	1.00	32.40	B	C
	ATOM	2555	NZ	LYS	174	13.087	-89.966	102.435	1.00	34.29	B	N
	ATOM	2556	C	LYS	174	9.344	-89.888	107.743	1.00	21.87	B	C
	ATOM	2557	O	LYS	174	9.709	-91.007	108.133	1.00	20.46	B	O
15	ATOM	2558	N	PHE	175	9.141	-88.862	108.563	1.00	21.53	B	N
	ATOM	2559	CA	PHE	175	9.291	-88.966	110.008	1.00	21.67	B	C
	ATOM	2560	CB	PHE	175	9.027	-87.599	110.643	1.00	21.39	B	C
	ATOM	2561	CG	PHE	175	8.820	-87.642	112.134	1.00	22.55	B	C
	ATOM	2562	CD1	PHE	175	9.878	-87.933	112.995	1.00	21.38	B	C
20	ATOM	2563	CD2	PHE	175	7.563	-87.373	112.679	1.00	22.64	B	C
	ATOM	2564	CE1	PHE	175	9.690	-87.953	114.374	1.00	21.89	B	C
	ATOM	2565	CE2	PHE	175	7.366	-87.393	114.061	1.00	23.00	B	C
	ATOM	2566	CZ	PHE	175	8.435	-87.684	114.910	1.00	22.35	B	C
	ATOM	2567	C	PHE	175	8.324	-89.999	110.581	1.00	21.68	B	C
25	ATOM	2568	O	PHE	175	8.718	-90.866	111.362	1.00	21.47	B	O
	ATOM	2569	N	THR	176	7.058	-89.910	110.188	1.00	22.73	B	N
	ATOM	2570	CA	THR	176	6.050	-90.838	110.686	1.00	24.75	B	C
	ATOM	2571	CB	THR	176	4.616	-90.434	110.230	1.00	25.26	B	C
	ATOM	2572	OG1	THR	176	4.482	-90.632	108.820	1.00	24.98	B	O
30	ATOM	2573	CG2	THR	176	4.331	-88.961	110.565	1.00	24.45	B	C
	ATOM	2574	C	THR	176	6.318	-92.285	110.257	1.00	25.69	B	C
	ATOM	2575	O	THR	176	6.172	-93.206	111.065	1.00	24.44	B	O
	ATOM	2576	N	LYS	177	6.737	-92.480	109.005	1.00	26.56	B	N
	ATOM	2577	CA	LYS	177	7.007	-93.824	108.489	1.00	28.90	B	C
35	ATOM	2578	CB	LYS	177	7.051	-93.805	106.958	1.00	29.06	B	C
	ATOM	2579	CG	LYS	177	5.721	-93.404	106.327	1.00	31.35	B	C
	ATOM	2580	CD	LYS	177	5.742	-93.550	104.815	1.00	33.93	B	C
	ATOM	2581	CE	LYS	177	4.452	-93.026	104.191	1.00	35.45	B	C
	ATOM	2582	NZ	LYS	177	3.233	-93.686	104.749	1.00	36.90	B	N
40	ATOM	2583	C	LYS	177	8.265	-94.500	109.047	1.00	29.97	B	C
	ATOM	2584	O	LYS	177	8.581	-95.632	108.681	1.00	30.08	B	O
	ATOM	2585	N	ASP	178	8.979	-93.799	109.924	1.00	30.95	B	N
	ATOM	2586	CA	ASP	178	10.171	-94.338	110.580	1.00	31.86	B	C
	ATOM	2587	CB	ASP	178	11.249	-93.255	110.695	1.00	33.44	B	C
45	ATOM	2588	CG	ASP	178	12.365	-93.427	109.689	1.00	35.31	B	C
	ATOM	2589	OD1	ASP	178	12.105	-93.955	108.587	1.00	36.42	B	O
	ATOM	2590	OD2	ASP	178	13.506	-93.018	109.994	1.00	37.36	B	O
	ATOM	2591	C	ASP	178	9.770	-94.814	111.986	1.00	31.51	B	C
	ATOM	2592	O	ASP	178	10.600	-95.282	112.760	1.00	31.62	B	O
50	ATOM	2593	N	LEU	179	8.485	-94.689	112.299	1.00	31.35	B	N
	ATOM	2594	CA	LEU	179	7.945	-95.083	113.593	1.00	31.19	B	C
	ATOM	2595	CB	LEU	179	7.050	-93.964	114.136	1.00	31.02	B	C
	ATOM	2596	CG	LEU	179	7.653	-92.737	114.840	1.00	31.99	B	C
	ATOM	2597	CD1	LEU	179	8.991	-92.337	114.255	1.00	31.68	B	C
	ATOM	2598	CD2	LEU	179	6.650	-91.592	114.747	1.00	31.31	B	C
55	ATOM	2599	C	LEU	179	7.127	-96.358	113.425	1.00	31.91	B	C
	ATOM	2600	O	LEU	179	6.002	-96.323	112.923	1.00	30.72	B	O
	ATOM	2601	N	PRO	180	7.682	-97.508	113.844	1.00	32.73	B	N
	ATOM	2602	CD	PRO	180	8.944	-97.731	114.565	1.00	32.93	B	C

-214-

	ATOM	2603	CA	PRO	180	6.932	-98.758	113.700	1.00	33.57	B	C
	ATOM	2604	CB	PRO	180	7.842	-99.789	114.374	1.00	33.58	B	C
	ATOM	2605	CG	PRO	180	8.636	-98.981	115.341	1.00	33.83	B	C
5	ATOM	2606	C	PRO	180	5.535	-98.679	114.319	1.00	34.14	B	C
	ATOM	2607	O	PRO	180	4.569	-99.203	113.763	1.00	33.78	B	O
	ATOM	2608	N	VAL	181	5.427	-98.002	115.457	1.00	34.64	B	N
	ATOM	2609	CA	VAL	181	4.140	-97.857	116.119	1.00	35.27	B	C
	ATOM	2610	CB	VAL	181	4.265	-97.083	117.441	1.00	35.75	B	C
10	ATOM	2611	CG1	VAL	181	2.911	-96.993	118.104	1.00	36.59	B	C
	ATOM	2612	CG2	VAL	181	5.258	-97.782	118.362	1.00	36.26	B	C
	ATOM	2613	C	VAL	181	3.148	-97.131	115.220	1.00	35.36	B	C
	ATOM	2614	O	VAL	181	1.986	-97.515	115.151	1.00	35.38	B	O
	ATOM	2615	N	PHE	182	3.599	-96.079	114.538	1.00	35.49	B	N
15	ATOM	2616	CA	PHE	182	2.726	-95.330	113.630	1.00	35.30	B	C
	ATOM	2617	CB	PHE	182	3.431	-94.071	113.117	1.00	33.92	B	C
	ATOM	2618	CG	PHE	182	2.597	-93.254	112.164	1.00	32.96	B	C
	ATOM	2619	CD1	PHE	182	1.647	-92.359	112.640	1.00	32.81	B	C
	ATOM	2620	CD2	PHE	182	2.760	-93.386	110.786	1.00	32.65	B	C
20	ATOM	2621	CE1	PHE	182	0.871	-91.604	111.759	1.00	32.61	B	C
	ATOM	2622	CE2	PHE	182	1.993	-92.640	109.897	1.00	32.30	B	C
	ATOM	2623	CZ	PHE	182	1.047	-91.746	110.382	1.00	32.70	B	C
	ATOM	2624	C	PHE	182	2.349	-96.212	112.439	1.00	36.18	B	C
	ATOM	2625	O	PHE	182	1.212	-96.183	111.966	1.00	35.72	B	O
25	ATOM	2626	N	ARG	183	3.315	-96.990	111.958	1.00	37.31	B	N
	ATOM	2627	CA	ARG	183	3.098	-97.885	110.830	1.00	39.17	B	C
	ATOM	2628	CB	ARG	183	4.427	-98.506	110.383	1.00	39.31	B	C
	ATOM	2629	CG	ARG	183	5.192	-97.668	109.381	1.00	39.52	B	C
	ATOM	2630	CD	ARG	183	6.380	-98.428	108.809	1.00	41.16	B	C
30	ATOM	2631	NE	ARG	183	7.596	-98.227	109.593	1.00	43.06	B	N
	ATOM	2632	CZ	ARG	183	8.263	-99.187	110.224	1.00	43.53	B	C
	ATOM	2633	NH1	ARG	183	7.840	-100.445	110.179	1.00	43.79	B	N
	ATOM	2634	NH2	ARG	183	9.370	-98.885	110.892	1.00	43.85	B	N
	ATOM	2635	C	ARG	183	2.094	-99.003	111.108	1.00	39.98	B	C
35	ATOM	2636	O	ARG	183	1.442	-99.493	110.187	1.00	39.52	B	O
	ATOM	2637	N	SER	184	1.962	-99.398	112.372	1.00	41.05	B	N
	ATOM	2638	CA	SER	184	1.054	-100.481	112.735	1.00	42.09	B	C
	ATOM	2639	CB	SER	184	1.462	-101.079	114.083	1.00	42.35	B	C
	ATOM	2640	OG	SER	184	1.270	-100.153	115.138	1.00	44.21	B	O
40	ATOM	2641	C	SER	184	-0.434	-100.137	112.765	1.00	42.40	B	C
	ATOM	2642	O	SER	184	-1.263	-101.034	112.899	1.00	42.68	B	O
	ATOM	2643	N	LEU	185	-0.788	-98.860	112.648	1.00	42.68	B	N
	ATOM	2644	CA	LEU	185	-2.201	-98.499	112.660	1.00	42.79	B	C
	ATOM	2645	CB	LEU	185	-2.441	-97.131	113.330	1.00	43.53	B	C
45	ATOM	2646	CG	LEU	185	-1.421	-96.007	113.534	1.00	44.02	B	C
	ATOM	2647	CD1	LEU	185	-2.140	-94.742	113.988	1.00	43.73	B	C
	ATOM	2648	CD2	LEU	185	-0.417	-96.404	114.589	1.00	44.56	B	C
	ATOM	2649	C	LEU	185	-2.831	-98.510	111.271	1.00	42.68	B	C
	ATOM	2650	O	LEU	185	-2.133	-98.457	110.258	1.00	42.19	B	O
50	ATOM	2651	N	PRO	186	-4.171	-98.598	111.209	1.00	42.84	B	N
	ATOM	2652	CD	PRO	186	-5.129	-98.602	112.327	1.00	42.91	B	C
	ATOM	2653	CA	PRO	186	-4.877	-98.615	109.926	1.00	43.29	B	C
	ATOM	2654	CB	PRO	186	-6.351	-98.617	110.337	1.00	43.26	B	C
	ATOM	2655	CG	PRO	186	-6.338	-97.972	111.696	1.00	43.70	B	C
55	ATOM	2656	C	PRO	186	-4.512	-97.421	109.054	1.00	43.49	B	C
	ATOM	2657	O	PRO	186	-4.262	-96.326	109.556	1.00	43.14	B	O
	ATOM	2658	N	ILE	187	-4.481	-97.650	107.747	1.00	43.61	B	N
	ATOM	2659	CA	ILE	187	-4.137	-96.613	106.784	1.00	43.56	B	C
	ATOM	2660	CB	ILE	187	-4.406	-97.082	105.337	1.00	43.82	B	C

-215-

5	ATOM	2661	CG2	ILE	187	-3.939	-96.018	104.353	1.00	43.79	B	C
	ATOM	2662	CG1	ILE	187	-3.667	-98.395	105.063	1.00	44.06	B	C
	ATOM	2663	CD1	ILE	187	-2.156	-98.288	105.188	1.00	44.66	B	C
	ATOM	2664	C	ILE	187	-4.916	-95.325	107.021	1.00	43.43	B	C
	ATOM	2665	O	ILE	187	-4.350	-94.232	106.975	1.00	42.67	B	O
10	ATOM	2666	N	GLU	188	-6.214	-95.451	107.272	1.00	43.55	B	N
	ATOM	2667	CA	GLU	188	-7.039	-94.273	107.496	1.00	44.32	B	C
	ATOM	2668	CB	GLU	188	-8.514	-94.658	107.582	1.00	45.62	B	C
	ATOM	2669	CG	GLU	188	-9.421	-93.446	107.496	1.00	48.84	B	C
	ATOM	2670	CD	GLU	188	-8.978	-92.471	106.406	1.00	50.12	B	C
15	ATOM	2671	OE1	GLU	188	-8.919	-92.875	105.223	1.00	51.29	B	O
	ATOM	2672	OE2	GLU	188	-8.684	-91.302	106.737	1.00	50.87	B	O
	ATOM	2673	C	GLU	188	-6.635	-93.469	108.735	1.00	43.37	B	C
	ATOM	2674	O	GLU	188	-6.760	-92.245	108.748	1.00	43.27	B	O
	ATOM	2675	N	ASP	189	-6.166	-94.149	109.776	1.00	42.33	B	N
20	ATOM	2676	CA	ASP	189	-5.720	-93.457	110.979	1.00	41.76	B	C
	ATOM	2677	CB	ASP	189	-5.510	-94.442	112.134	1.00	42.89	B	C
	ATOM	2678	CG	ASP	189	-6.811	-94.832	112.806	1.00	44.75	B	C
	ATOM	2679	OD1	ASP	189	-6.768	-95.471	113.879	1.00	46.20	B	O
	ATOM	2680	OD2	ASP	189	-7.882	-94.498	112.258	1.00	45.42	B	O
25	ATOM	2681	C	ASP	189	-4.417	-92.718	110.683	1.00	40.38	B	C
	ATOM	2682	O	ASP	189	-4.237	-91.578	111.102	1.00	40.12	B	O
	ATOM	2683	N	GLN	190	-3.515	-93.369	109.955	1.00	39.17	B	N
	ATOM	2684	CA	GLN	190	-2.241	-92.757	109.592	1.00	38.44	B	C
	ATOM	2685	CB	GLN	190	-1.416	-93.702	108.725	1.00	37.85	B	C
30	ATOM	2686	CG	GLN	190	-1.088	-95.032	109.373	1.00	38.72	B	C
	ATOM	2687	CD	GLN	190	-0.103	-95.854	108.560	1.00	38.85	B	C
	ATOM	2688	OE1	GLN	190	0.060	-97.054	108.789	1.00	38.95	B	O
	ATOM	2689	NE2	GLN	190	0.567	-95.209	107.611	1.00	39.18	B	N
	ATOM	2690	C	GLN	190	-2.486	-91.468	108.822	1.00	37.77	B	C
35	ATOM	2691	O	GLN	190	-1.846	-90.451	109.077	1.00	38.02	B	O
	ATOM	2692	N	ILE	191	-3.418	-91.521	107.877	1.00	37.50	B	N
	ATOM	2693	CA	ILE	191	-3.761	-90.364	107.061	1.00	37.36	B	C
	ATOM	2694	CB	ILE	191	-4.787	-90.737	105.964	1.00	38.55	B	C
	ATOM	2695	CG2	ILE	191	-5.031	-89.548	105.059	1.00	38.60	B	C
40	ATOM	2696	CG1	ILE	191	-4.278	-91.921	105.138	1.00	39.51	B	C
	ATOM	2697	CD1	ILE	191	-3.011	-91.637	104.353	1.00	41.55	B	C
	ATOM	2698	C	ILE	191	-4.356	-89.252	107.919	1.00	36.51	B	C
	ATOM	2699	O	ILE	191	-3.955	-88.094	107.804	1.00	36.70	B	O
	ATOM	2700	N	SER	192	-5.312	-89.606	108.776	1.00	35.03	B	N
45	ATOM	2701	CA	SER	192	-5.959	-88.628	109.646	1.00	34.26	B	C
	ATOM	2702	CB	SER	192	-7.086	-89.286	110.446	1.00	34.74	B	C
	ATOM	2703	OG	SER	192	-8.107	-89.757	109.586	1.00	35.76	B	O
	ATOM	2704	C	SER	192	-4.982	-87.956	110.608	1.00	32.87	B	C
	ATOM	2705	O	SER	192	-5.078	-86.753	110.853	1.00	31.92	B	O
50	ATOM	2706	N	LEU	193	-4.054	-88.732	111.160	1.00	31.50	B	N
	ATOM	2707	CA	LEU	193	-3.072	-88.183	112.085	1.00	30.70	B	C
	ATOM	2708	CB	LEU	193	-2.295	-89.305	112.786	1.00	29.93	B	C
	ATOM	2709	CG	LEU	193	-3.072	-90.217	113.746	1.00	29.73	B	C
	ATOM	2710	CD1	LEU	193	-2.099	-91.157	114.450	1.00	29.19	B	C
55	ATOM	2711	CD2	LEU	193	-3.831	-89.379	114.765	1.00	27.88	B	C
	ATOM	2712	C	LEU	193	-2.107	-87.268	111.337	1.00	30.76	B	C
	ATOM	2713	O	LEU	193	-1.809	-86.164	111.789	1.00	29.84	B	O
	ATOM	2714	N	LEU	194	-1.625	-87.725	110.187	1.00	31.33	B	N
	ATOM	2715	CA	LEU	194	-0.706	-86.924	109.389	1.00	32.09	B	C
	ATOM	2716	CB	LEU	194	-0.297	-87.711	108.142	1.00	32.64	B	C
	ATOM	2717	CG	LEU	194	0.922	-87.259	107.333	1.00	34.23	B	C
	ATOM	2718	CD1	LEU	194	0.579	-85.995	106.557	1.00	35.50	B	C

-216-

	ATOM	2719	CD2	LEU	194	2.116	-87.032	108.260	1.00	33.53	B	C
	ATOM	2720	C	LEU	194	-1.370	-85.589	109.017	1.00	32.06	B	C
	ATOM	2721	O	LEU	194	-0.831	-84.523	109.303	1.00	31.90	B	O
5	ATOM	2722	N	LYS	195	-2.549	-85.651	108.402	1.00	32.21	B	N
	ATOM	2723	CA	LYS	195	-3.289	-84.448	108.014	1.00	32.26	B	C
	ATOM	2724	CB	LYS	195	-4.643	-84.832	107.404	1.00	34.49	B	C
	ATOM	2725	CG	LYS	195	-4.562	-85.427	106.005	1.00	36.99	B	C
	ATOM	2726	CD	LYS	195	-5.851	-86.146	105.619	1.00	38.55	B	C
10	ATOM	2727	CE	LYS	195	-7.061	-85.223	105.632	1.00	39.77	B	C
	ATOM	2728	NZ	LYS	195	-8.275	-85.939	105.131	1.00	41.50	B	N
	ATOM	2729	C	LYS	195	-3.541	-83.517	109.197	1.00	31.45	B	C
	ATOM	2730	O	LYS	195	-3.455	-82.292	109.079	1.00	30.78	B	O
	ATOM	2731	N	GLY	196	-3.862	-84.105	110.339	1.00	29.85	B	N
15	ATOM	2732	CA	GLY	196	-4.141	-83.303	111.509	1.00	28.37	B	C
	ATOM	2733	C	GLY	196	-2.946	-82.676	112.195	1.00	26.84	B	C
	ATOM	2734	O	GLY	196	-3.090	-81.621	112.806	1.00	26.88	B	O
	ATOM	2735	N	ALA	197	-1.768	-83.284	112.085	1.00	25.28	B	N
	ATOM	2736	CA	ALA	197	-0.596	-82.751	112.785	1.00	23.92	B	C
20	ATOM	2737	CB	ALA	197	-0.125	-83.776	113.816	1.00	23.40	B	C
	ATOM	2738	C	ALA	197	0.608	-82.269	111.978	1.00	22.01	B	C
	ATOM	2739	O	ALA	197	1.536	-81.706	112.550	1.00	20.56	B	O
	ATOM	2740	N	ALA	198	0.606	-82.483	110.668	1.00	20.97	B	N
	ATOM	2741	CA	ALA	198	1.737	-82.073	109.836	1.00	20.46	B	C
25	ATOM	2742	CB	ALA	198	1.406	-82.284	108.349	1.00	20.75	B	C
	ATOM	2743	C	ALA	198	2.188	-80.631	110.071	1.00	19.62	B	C
	ATOM	2744	O	ALA	198	3.359	-80.381	110.365	1.00	19.14	B	O
	ATOM	2745	N	VAL	199	1.262	-79.689	109.935	1.00	19.02	B	N
	ATOM	2746	CA	VAL	199	1.566	-78.276	110.125	1.00	19.01	B	C
30	ATOM	2747	CB	VAL	199	0.365	-77.401	109.738	1.00	19.49	B	C
	ATOM	2748	CG1	VAL	199	0.658	-75.938	110.073	1.00	18.87	B	C
	ATOM	2749	CG2	VAL	199	0.074	-77.563	108.243	1.00	19.44	B	C
	ATOM	2750	C	VAL	199	1.986	-77.946	111.555	1.00	18.82	B	C
	ATOM	2751	O	VAL	199	2.856	-77.104	111.766	1.00	19.08	B	O
35	ATOM	2752	N	GLU	200	1.369	-78.605	112.531	1.00	17.97	B	N
	ATOM	2753	CA	GLU	200	1.713	-78.389	113.934	1.00	18.43	B	C
	ATOM	2754	CB	GLU	200	0.751	-79.152	114.850	1.00	18.15	B	C
	ATOM	2755	CG	GLU	200	-0.600	-78.479	115.030	1.00	20.07	B	C
	ATOM	2756	CD	GLU	200	-1.570	-79.307	115.866	1.00	21.56	B	C
40	ATOM	2757	OE1	GLU	200	-1.123	-80.050	116.765	1.00	21.43	B	O
	ATOM	2758	OE2	GLU	200	-2.785	-79.197	115.630	1.00	22.35	B	O
	ATOM	2759	C	GLU	200	3.138	-78.854	114.202	1.00	17.94	B	C
	ATOM	2760	O	GLU	200	3.920	-78.148	114.830	1.00	18.17	B	O
	ATOM	2761	N	ILE	201	3.469	-80.047	113.716	1.00	17.97	B	N
45	ATOM	2762	CA	ILE	201	4.799	-80.612	113.897	1.00	17.91	B	C
	ATOM	2763	CB	ILE	201	4.840	-82.051	113.335	1.00	18.26	B	C
	ATOM	2764	CG2	ILE	201	6.266	-82.572	113.260	1.00	17.92	B	C
	ATOM	2765	CG1	ILE	201	3.986	-82.953	114.233	1.00	17.28	B	C
	ATOM	2766	CD1	ILE	201	3.815	-84.368	113.701	1.00	18.61	B	C
50	ATOM	2767	C	ILE	201	5.869	-79.731	113.255	1.00	17.32	B	C
	ATOM	2768	O	ILE	201	6.953	-79.547	113.815	1.00	18.72	B	O
	ATOM	2769	N	CYS	202	5.567	-79.165	112.095	1.00	16.54	B	N
	ATOM	2770	CA	CYS	202	6.522	-78.282	111.434	1.00	16.29	B	C
	ATOM	2771	CB	CYS	202	5.996	-77.845	110.062	1.00	16.39	B	C
	ATOM	2772	SG	CYS	202	5.924	-79.183	108.838	1.00	16.45	B	S
55	ATOM	2773	C	CYS	202	6.822	-77.049	112.295	1.00	15.32	B	C
	ATOM	2774	O	CYS	202	7.968	-76.624	112.386	1.00	14.15	B	O
	ATOM	2775	N	HIS	203	5.806	-76.463	112.924	1.00	15.37	B	N
	ATOM	2776	CA	HIS	203	6.061	-75.290	113.768	1.00	15.80	B	C

-217-

5	ATOM	2777	CB	HIS	203	4.750	-74.610	114.164	1.00	15.84	B	C
	ATOM	2778	CG	HIS	203	4.173	-73.757	113.076	1.00	15.00	B	C
	ATOM	2779	CD2	HIS	203	3.148	-73.977	112.221	1.00	15.47	B	C
	ATOM	2780	ND1	HIS	203	4.719	-72.545	112.714	1.00	15.56	B	N
	ATOM	2781	CE1	HIS	203	4.058	-72.056	111.681	1.00	15.06	B	C
	ATOM	2782	NE2	HIS	203	3.100	-72.906	111.361	1.00	15.27	B	N
	ATOM	2783	C	HIS	203	6.886	-75.646	115.003	1.00	15.74	B	C
	ATOM	2784	O	HIS	203	7.738	-74.867	115.422	1.00	16.61	B	O
10	ATOM	2785	N	ILE	204	6.643	-76.818	115.581	1.00	14.51	B	N
	ATOM	2786	CA	ILE	204	7.421	-77.263	116.734	1.00	15.77	B	C
	ATOM	2787	CB	ILE	204	6.914	-78.643	117.266	1.00	14.78	B	C
	ATOM	2788	CG2	ILE	204	7.885	-79.192	118.305	1.00	14.01	B	C
15	ATOM	2789	CG1	ILE	204	5.496	-78.495	117.853	1.00	14.35	B	C
	ATOM	2790	CD1	ILE	204	4.849	-79.812	118.317	1.00	11.99	B	C
	ATOM	2791	C	ILE	204	8.890	-77.404	116.303	1.00	15.99	B	C
	ATOM	2792	O	ILE	204	9.803	-76.963	117.001	1.00	14.96	B	O
	ATOM	2793	N	VAL	205	9.108	-78.011	115.140	1.00	16.33	B	N
20	ATOM	2794	CA	VAL	205	10.463	-78.208	114.623	1.00	18.21	B	C
	ATOM	2795	CB	VAL	205	10.455	-79.139	113.402	1.00	17.84	B	C
	ATOM	2796	CG1	VAL	205	11.796	-79.058	112.671	1.00	17.90	B	C
	ATOM	2797	CG2	VAL	205	10.169	-80.565	113.862	1.00	18.55	B	C
	ATOM	2798	C	VAL	205	11.153	-76.906	114.242	1.00	17.83	B	C
	ATOM	2799	O	VAL	205	12.317	-76.698	114.550	1.00	17.35	B	O
25	ATOM	2800	N	LEU	206	10.434	-76.027	113.565	1.00	18.27	B	N
	ATOM	2801	CA	LEU	206	11.006	-74.745	113.167	1.00	19.32	B	C
	ATOM	2802	CB	LEU	206	10.051	-74.037	112.202	1.00	19.42	B	C
	ATOM	2803	CG	LEU	206	10.452	-73.904	110.727	1.00	21.56	B	C
	ATOM	2804	CD1	LEU	206	11.505	-74.932	110.327	1.00	21.35	B	C
30	ATOM	2805	CD2	LEU	206	9.196	-74.031	109.890	1.00	21.44	B	C
	ATOM	2806	C	LEU	206	11.318	-73.827	114.357	1.00	18.20	B	C
	ATOM	2807	O	LEU	206	12.121	-72.902	114.238	1.00	17.70	B	O
	ATOM	2808	N	ASN	207	10.688	-74.079	115.500	1.00	17.51	B	N
	ATOM	2809	CA	ASN	207	10.918	-73.251	116.680	1.00	17.40	B	C
35	ATOM	2810	CB	ASN	207	10.124	-73.774	117.874	1.00	15.99	B	C
	ATOM	2811	CG	ASN	207	10.184	-72.828	119.073	1.00	16.60	B	C
	ATOM	2812	OD1	ASN	207	10.860	-73.101	120.068	1.00	15.13	B	O
	ATOM	2813	ND2	ASN	207	9.485	-71.701	118.970	1.00	13.67	B	N
	ATOM	2814	C	ASN	207	12.387	-73.144	117.061	1.00	18.07	B	C
40	ATOM	2815	O	ASN	207	12.804	-72.133	117.621	1.00	17.57	B	O
	ATOM	2816	N	THR	208	13.172	-74.179	116.764	1.00	18.22	B	N
	ATOM	2817	CA	THR	208	14.595	-74.147	117.080	1.00	20.72	B	C
	ATOM	2818	CB	THR	208	15.258	-75.534	116.894	1.00	21.89	B	C
	ATOM	2819	OG1	THR	208	15.018	-76.015	115.565	1.00	23.70	B	O
45	ATOM	2820	CG2	THR	208	14.676	-76.540	117.906	1.00	22.78	B	C
	ATOM	2821	C	THR	208	15.366	-73.105	116.268	1.00	20.46	B	C
	ATOM	2822	O	THR	208	16.501	-72.785	116.599	1.00	21.62	B	O
	ATOM	2823	N	THR	209	14.760	-72.568	115.212	1.00	19.69	B	N
	ATOM	2824	CA	THR	209	15.423	-71.536	114.413	1.00	19.16	B	C
50	ATOM	2825	CB	THR	209	15.153	-71.700	112.899	1.00	18.90	B	C
	ATOM	2826	OG1	THR	209	13.776	-71.401	112.619	1.00	17.30	B	O
	ATOM	2827	CG2	THR	209	15.474	-73.121	112.451	1.00	18.39	B	C
	ATOM	2828	C	THR	209	14.944	-70.134	114.804	1.00	19.06	B	C
	ATOM	2829	O	THR	209	15.456	-69.144	114.299	1.00	17.85	B	O
55	ATOM	2830	N	PHE	210	13.962	-70.053	115.698	1.00	18.89	B	N
	ATOM	2831	CA	PHE	210	13.429	-68.760	116.112	1.00	20.27	B	C
	ATOM	2832	CB	PHE	210	12.107	-68.936	116.877	1.00	18.70	B	C
	ATOM	2833	CG	PHE	210	11.307	-67.661	117.020	1.00	18.90	B	C
	ATOM	2834	CD1	PHE	210	10.694	-67.081	115.914	1.00	18.35	B	C

-218-

5	ATOM	2835	CD2	PHE	210	11.161	-67.046	118.263	1.00	19.05	B	C
	ATOM	2836	CE1	PHE	210	9.945	-65.909	116.039	1.00	18.54	B	C
	ATOM	2837	CE2	PHE	210	10.409	-65.865	118.401	1.00	19.42	B	C
	ATOM	2838	CZ	PHE	210	9.802	-65.299	117.286	1.00	18.58	B	C
	ATOM	2839	C	PHE	210	14.411	-68.002	116.986	1.00	20.77	B	C
10	ATOM	2840	O	PHE	210	14.847	-68.498	118.021	1.00	20.70	B	O
	ATOM	2841	N	CYS	211	14.759	-66.794	116.565	1.00	22.21	B	N
	ATOM	2842	CA	CYS	211	15.674	-65.953	117.327	1.00	24.26	B	C
	ATOM	2843	CB	CYS	211	16.575	-65.155	116.391	1.00	24.98	B	C
	ATOM	2844	SG	CYS	211	17.664	-64.026	117.267	1.00	27.94	B	S
15	ATOM	2845	C	CYS	211	14.824	-64.996	118.148	1.00	25.17	B	C
	ATOM	2846	O	CYS	211	14.060	-64.209	117.586	1.00	24.50	B	O
	ATOM	2847	N	LEU	212	14.950	-65.076	119.471	1.00	25.78	B	N
	ATOM	2848	CA	LEU	212	14.173	-64.229	120.375	1.00	27.77	B	C
	ATOM	2849	CB	LEU	212	14.396	-64.652	121.830	1.00	26.74	B	C
20	ATOM	2850	CG	LEU	212	13.735	-65.968	122.237	1.00	26.59	B	C
	ATOM	2851	CD1	LEU	212	14.046	-66.279	123.700	1.00	26.25	B	C
	ATOM	2852	CD2	LEU	212	12.235	-65.863	122.014	1.00	24.89	B	C
	ATOM	2853	C	LEU	212	14.448	-62.739	120.253	1.00	28.72	B	C
	ATOM	2854	O	LEU	212	13.521	-61.931	120.271	1.00	29.38	B	O
25	ATOM	2855	N	GLN	213	15.720	-62.379	120.140	1.00	30.42	B	N
	ATOM	2856	CA	GLN	213	16.108	-60.982	120.027	1.00	32.34	B	C
	ATOM	2857	CB	GLN	213	17.631	-60.869	119.893	1.00	35.12	B	C
	ATOM	2858	CG	GLN	213	18.122	-59.462	119.576	1.00	38.96	B	C
	ATOM	2859	CD	GLN	213	18.458	-58.655	120.817	1.00	41.53	B	C
30	ATOM	2860	OE1	GLN	213	19.566	-58.754	121.357	1.00	42.98	B	O
	ATOM	2861	NE2	GLN	213	17.500	-57.858	121.284	1.00	42.35	B	N
	ATOM	2862	C	GLN	213	15.453	-60.262	118.846	1.00	32.03	B	C
	ATOM	2863	O	GLN	213	15.005	-59.126	118.986	1.00	32.80	B	O
	ATOM	2864	N	THR	214	15.390	-60.919	117.691	1.00	30.84	B	N
35	ATOM	2865	CA	THR	214	14.828	-60.288	116.497	1.00	29.82	B	C
	ATOM	2866	CB	THR	214	15.808	-60.393	115.316	1.00	29.30	B	C
	ATOM	2867	OG1	THR	214	16.083	-61.773	115.049	1.00	28.95	B	O
	ATOM	2868	CG2	THR	214	17.108	-59.679	115.636	1.00	30.14	B	C
	ATOM	2869	C	THR	214	13.472	-60.792	116.009	1.00	29.36	B	C
40	ATOM	2870	O	THR	214	12.941	-60.264	115.032	1.00	28.67	B	O
	ATOM	2871	N	GLN	215	12.918	-61.805	116.670	1.00	28.97	B	N
	ATOM	2872	CA	GLN	215	11.623	-62.361	116.273	1.00	29.50	B	C
	ATOM	2873	CB	GLN	215	10.533	-61.284	116.375	1.00	30.88	B	C
	ATOM	2874	CG	GLN	215	10.336	-60.704	117.764	1.00	33.91	B	C
45	ATOM	2875	CD	GLN	215	9.754	-61.711	118.726	1.00	35.71	B	C
	ATOM	2876	OE1	GLN	215	8.651	-62.221	118.513	1.00	37.61	B	O
	ATOM	2877	NE2	GLN	215	10.492	-62.010	119.793	1.00	36.76	B	N
	ATOM	2878	C	GLN	215	11.670	-62.890	114.834	1.00	28.46	B	C
	ATOM	2879	O	GLN	215	10.696	-62.774	114.093	1.00	28.52	B	O
50	ATOM	2880	N	ASN	216	12.801	-63.465	114.442	1.00	26.98	B	N
	ATOM	2881	CA	ASN	216	12.960	-63.990	113.092	1.00	25.74	B	C
	ATOM	2882	CB	ASN	216	14.085	-63.250	112.363	1.00	27.52	B	C
	ATOM	2883	CG	ASN	216	13.770	-61.786	112.093	1.00	28.70	B	C
	ATOM	2884	OD1	ASN	216	14.664	-61.022	111.749	1.00	27.69	B	O
55	ATOM	2885	ND2	ASN	216	12.503	-61.394	112.228	1.00	29.92	B	N
	ATOM	2886	C	ASN	216	13.326	-65.461	113.125	1.00	24.08	B	C
	ATOM	2887	O	ASN	216	13.849	-65.945	114.119	1.00	22.97	B	O
	ATOM	2888	N	PHE	217	13.049	-66.164	112.032	1.00	22.85	B	N
	ATOM	2889	CA	PHE	217	13.410	-67.568	111.906	1.00	22.30	B	C
	ATOM	2890	CB	PHE	217	12.323	-68.373	111.195	1.00	20.84	B	C
	ATOM	2891	CG	PHE	217	11.052	-68.503	111.975	1.00	20.02	B	C
	ATOM	2892	CD1	PHE	217	10.095	-67.494	111.948	1.00	19.19	B	C

-219-

5	ATOM	2893	CD2	PHE	217	10.805	-69.644	112.733	1.00	19.92	B	C
	ATOM	2894	CE1	PHE	217	8.909	-67.622	112.664	1.00	18.54	B	C
	ATOM	2895	CE2	PHE	217	9.620	-69.780	113.453	1.00	19.66	B	C
	ATOM	2896	CZ	PHE	217	8.672	-68.763	113.415	1.00	19.48	B	C
	ATOM	2897	C	PHE	217	14.676	-67.588	111.057	1.00	22.98	B	C
10	ATOM	2898	O	PHE	217	14.652	-67.184	109.895	1.00	21.70	B	O
	ATOM	2899	N	LEU	218	15.777	-68.046	111.645	1.00	23.53	B	N
	ATOM	2900	CA	LEU	218	17.066	-68.114	110.957	1.00	24.87	B	C
	ATOM	2901	CB	LEU	218	18.210	-67.785	111.930	1.00	26.08	B	C
	ATOM	2902	CG	LEU	218	18.380	-66.339	112.436	1.00	27.99	B	C
15	ATOM	2903	CD1	LEU	218	17.118	-65.845	113.126	1.00	27.86	B	C
	ATOM	2904	CD2	LEU	218	19.555	-66.279	113.413	1.00	27.96	B	C
	ATOM	2905	C	LEU	218	17.260	-69.510	110.383	1.00	25.07	B	C
	ATOM	2906	O	LEU	218	17.539	-70.458	111.115	1.00	25.64	B	O
	ATOM	2907	N	CYS	219	17.105	-69.631	109.069	1.00	24.23	B	N
20	ATOM	2908	CA	CYS	219	17.244	-70.918	108.396	1.00	23.85	B	C
	ATOM	2909	CB	CYS	219	15.935	-71.263	107.674	1.00	22.48	B	C
	ATOM	2910	SG	CYS	219	14.462	-71.225	108.747	1.00	19.92	B	S
	ATOM	2911	C	CYS	219	18.406	-70.868	107.398	1.00	24.42	B	C
	ATOM	2912	O	CYS	219	18.231	-70.505	106.227	1.00	22.82	B	O
25	ATOM	2913	N	GLY	220	19.590	-71.252	107.870	1.00	25.23	B	N
	ATOM	2914	CA	GLY	220	20.764	-71.214	107.021	1.00	24.90	B	C
	ATOM	2915	C	GLY	220	20.996	-69.754	106.695	1.00	24.77	B	C
	ATOM	2916	O	GLY	220	21.031	-68.922	107.601	1.00	24.69	B	O
	ATOM	2917	N	PRO	221	21.152	-69.401	105.412	1.00	24.50	B	N
30	ATOM	2918	CD	PRO	221	21.305	-70.265	104.229	1.00	23.93	B	C
	ATOM	2919	CA	PRO	221	21.374	-67.993	105.060	1.00	24.42	B	C
	ATOM	2920	CB	PRO	221	22.053	-68.090	103.699	1.00	23.72	B	C
	ATOM	2921	CG	PRO	221	21.356	-69.247	103.085	1.00	23.75	B	C
	ATOM	2922	C	PRO	221	20.073	-67.181	104.995	1.00	23.85	B	C
35	ATOM	2923	O	PRO	221	20.108	-65.967	104.811	1.00	23.61	B	O
	ATOM	2924	N	LEU	222	18.935	-67.858	105.153	1.00	22.94	B	N
	ATOM	2925	CA	LEU	222	17.627	-67.209	105.084	1.00	22.55	B	C
	ATOM	2926	CB	LEU	222	16.595	-68.162	104.478	1.00	20.79	B	C
	ATOM	2927	CG	LEU	222	16.913	-68.732	103.100	1.00	19.76	B	C
40	ATOM	2928	CD1	LEU	222	15.742	-69.560	102.623	1.00	20.37	B	C
	ATOM	2929	CD2	LEU	222	17.199	-67.594	102.122	1.00	20.15	B	C
	ATOM	2930	C	LEU	222	17.093	-66.695	106.415	1.00	22.84	B	C
	ATOM	2931	O	LEU	222	17.341	-67.275	107.473	1.00	23.24	B	O
	ATOM	2932	N	ARG	223	16.343	-65.603	106.333	1.00	22.89	B	N
45	ATOM	2933	CA	ARG	223	15.733	-64.960	107.485	1.00	24.01	B	C
	ATOM	2934	CB	ARG	223	16.451	-63.650	107.782	1.00	26.47	B	C
	ATOM	2935	CG	ARG	223	15.718	-62.751	108.768	1.00	31.77	B	C
	ATOM	2936	CD	ARG	223	16.177	-61.310	108.616	1.00	35.27	B	C
	ATOM	2937	NE	ARG	223	15.723	-60.734	107.349	1.00	38.31	B	N
50	ATOM	2938	CZ	ARG	223	16.314	-59.714	106.740	1.00	39.39	B	C
	ATOM	2939	NH1	ARG	223	17.389	-59.158	107.279	1.00	41.22	B	N
	ATOM	2940	NH2	ARG	223	15.824	-59.240	105.600	1.00	40.79	B	N
	ATOM	2941	C	ARG	223	14.265	-64.663	107.183	1.00	23.59	B	C
	ATOM	2942	O	ARG	223	13.964	-63.869	106.287	1.00	22.38	B	O
55	ATOM	2943	N	TYR	224	13.359	-65.296	107.930	1.00	22.01	B	N
	ATOM	2944	CA	TYR	224	11.921	-65.086	107.742	1.00	21.48	B	C
	ATOM	2945	CB	TYR	224	11.163	-66.411	107.718	1.00	20.04	B	C
	ATOM	2946	CG	TYR	224	11.572	-67.355	106.615	1.00	19.13	B	C
	ATOM	2947	CD1	TYR	224	12.511	-68.361	106.851	1.00	17.91	B	C
	ATOM	2948	CE1	TYR	224	12.886	-69.240	105.848	1.00	18.05	B	C
	ATOM	2949	CD2	TYR	224	11.019	-67.249	105.338	1.00	17.45	B	C
	ATOM	2950	CE2	TYR	224	11.392	-68.124	104.319	1.00	17.93	B	C

-220-

5	ATOM	2951	CZ	TYR	224	12.328	-69.118	104.587	1.00	17.71	B	C
	ATOM	2952	OH	TYR	224	12.714	-69.995	103.606	1.00	17.71	B	O
	ATOM	2953	C	TYR	224	11.352	-64.239	108.872	1.00	21.91	B	C
	ATOM	2954	O	TYR	224	11.619	-64.502	110.043	1.00	21.72	B	O
	ATOM	2955	N	THR	225	10.556	-63.238	108.509	1.00	21.54	B	N
10	ATOM	2956	CA	THR	225	9.942	-62.340	109.478	1.00	21.65	B	C
	ATOM	2957	CB	THR	225	10.335	-60.874	109.202	1.00	23.19	B	C
	ATOM	2958	OG1	THR	225	9.847	-60.492	107.912	1.00	22.96	B	O
	ATOM	2959	CG2	THR	225	11.853	-60.695	109.232	1.00	23.33	B	C
	ATOM	2960	C	THR	225	8.418	-62.421	109.416	1.00	20.84	B	C
15	ATOM	2961	O	THR	225	7.849	-63.042	108.513	1.00	19.99	B	O
	ATOM	2962	N	ILE	226	7.764	-61.773	110.376	1.00	19.42	B	N
	ATOM	2963	CA	ILE	226	6.311	-61.746	110.430	1.00	18.00	B	C
	ATOM	2964	CB	ILE	226	5.837	-61.101	111.768	1.00	17.71	B	C
	ATOM	2965	CG2	ILE	226	6.223	-59.625	111.813	1.00	16.28	B	C
20	ATOM	2966	CG1	ILE	226	4.334	-61.306	111.963	1.00	15.92	B	C
	ATOM	2967	CD1	ILE	226	3.849	-60.925	113.363	1.00	13.01	B	C
	ATOM	2968	C	ILE	226	5.762	-60.988	109.207	1.00	18.53	B	C
	ATOM	2969	O	ILE	226	4.646	-61.249	108.754	1.00	17.76	B	O
	ATOM	2970	N	GLU	227	6.555	-60.071	108.649	1.00	18.32	B	N
25	ATOM	2971	CA	GLU	227	6.119	-59.335	107.468	1.00	19.11	B	C
	ATOM	2972	CB	GLU	227	7.110	-58.221	107.103	1.00	20.59	B	C
	ATOM	2973	CG	GLU	227	7.032	-56.939	107.959	1.00	20.58	B	C
	ATOM	2974	CD	GLU	227	7.477	-57.143	109.396	1.00	21.61	B	C
	ATOM	2975	OE1	GLU	227	8.490	-57.839	109.617	1.00	23.10	B	O
30	ATOM	2976	OE2	GLU	227	6.825	-56.596	110.308	1.00	22.37	B	O
	ATOM	2977	C	GLU	227	5.960	-60.277	106.273	1.00	18.86	B	C
	ATOM	2978	O	GLU	227	5.114	-60.049	105.416	1.00	18.23	B	O
	ATOM	2979	N	ASP	228	6.767	-61.334	106.199	1.00	18.37	B	N
	ATOM	2980	CA	ASP	228	6.631	-62.255	105.071	1.00	18.69	B	C
35	ATOM	2981	CB	ASP	228	7.733	-63.333	105.088	1.00	18.93	B	C
	ATOM	2982	CG	ASP	228	9.135	-62.743	104.950	1.00	19.98	B	C
	ATOM	2983	OD1	ASP	228	9.348	-61.929	104.031	1.00	20.95	B	O
	ATOM	2984	OD2	ASP	228	10.025	-63.094	105.754	1.00	19.87	B	O
	ATOM	2985	C	ASP	228	5.239	-62.899	105.102	1.00	18.01	B	C
40	ATOM	2986	O	ASP	228	4.593	-63.045	104.064	1.00	18.44	B	O
	ATOM	2987	N	GLY	229	4.776	-63.281	106.289	1.00	17.20	B	N
	ATOM	2988	CA	GLY	229	3.449	-63.866	106.392	1.00	17.52	B	C
	ATOM	2989	C	GLY	229	2.371	-62.845	106.035	1.00	17.70	B	C
	ATOM	2990	O	GLY	229	1.411	-63.157	105.330	1.00	18.08	B	O
45	ATOM	2991	N	ALA	230	2.532	-61.614	106.510	1.00	17.31	B	N
	ATOM	2992	CA	ALA	230	1.561	-60.557	106.237	1.00	17.67	B	C
	ATOM	2993	CB	ALA	230	1.921	-59.312	107.031	1.00	17.60	B	C
	ATOM	2994	C	ALA	230	1.457	-60.213	104.749	1.00	18.51	B	C
	ATOM	2995	O	ALA	230	0.367	-59.982	104.231	1.00	17.21	B	O
50	ATOM	2996	N	ARG	231	2.594	-60.177	104.060	1.00	19.86	B	N
	ATOM	2997	CA	ARG	231	2.599	-59.844	102.643	1.00	20.24	B	C
	ATOM	2998	CB	ARG	231	4.027	-59.549	102.173	1.00	21.54	B	C
	ATOM	2999	CG	ARG	231	4.665	-58.322	102.843	1.00	23.12	B	C
	ATOM	3000	CD	ARG	231	3.911	-57.026	102.506	1.00	23.94	B	C
55	ATOM	3001	NE	ARG	231	4.022	-56.665	101.092	1.00	25.20	B	N
	ATOM	3002	CZ	ARG	231	5.058	-56.026	100.553	1.00	25.86	B	C
	ATOM	3003	NH1	ARG	231	6.090	-55.661	101.301	1.00	25.92	B	N
	ATOM	3004	NH2	ARG	231	5.064	-55.746	99.258	1.00	26.68	B	N
	ATOM	3005	C	ARG	231	1.963	-60.919	101.765	1.00	20.12	B	C
	ATOM	3006	O	ARG	231	1.561	-60.632	100.640	1.00	19.52	B	O
	ATOM	3007	N	VAL	232	1.865	-62.153	102.256	1.00	19.90	B	N
	ATOM	3008	CA	VAL	232	1.239	-63.195	101.450	1.00	19.34	B	C

-221-

	ATOM	3009	CB	VAL	232	1.927	-64.592	101.612	1.00	20.66	B	C
	ATOM	3010	CG1	VAL	232	3.413	-64.476	101.307	1.00	19.33	B	C
	ATOM	3011	CG2	VAL	232	1.671	-65.169	103.017	1.00	18.79	B	C
5	ATOM	3012	C	VAL	232	-0.245	-63.330	101.779	1.00	19.07	B	C
	ATOM	3013	O	VAL	232	-0.926	-64.191	101.230	1.00	17.55	B	O
	ATOM	3014	N	GLY	233	-0.745	-62.486	102.680	1.00	19.78	B	N
	ATOM	3015	CA	GLY	233	-2.161	-62.535	103.008	1.00	20.41	B	C
	ATOM	3016	C	GLY	233	-2.643	-62.915	104.397	1.00	21.13	B	C
10	ATOM	3017	O	GLY	233	-3.805	-62.655	104.719	1.00	21.49	B	O
	ATOM	3018	N	PHE	234	-1.806	-63.541	105.223	1.00	20.51	B	N
	ATOM	3019	CA	PHE	234	-2.268	-63.905	106.563	1.00	20.56	B	C
	ATOM	3020	CB	PHE	234	-1.205	-64.706	107.326	1.00	20.73	B	C
	ATOM	3021	CG	PHE	234	-0.998	-66.103	106.810	1.00	20.24	B	C
15	ATOM	3022	CD1	PHE	234	0.169	-66.441	106.135	1.00	19.02	B	C
	ATOM	3023	CD2	PHE	234	-1.956	-67.093	107.035	1.00	19.67	B	C
	ATOM	3024	CE1	PHE	234	0.386	-67.747	105.695	1.00	19.63	B	C
	ATOM	3025	CE2	PHE	234	-1.748	-68.403	106.597	1.00	19.47	B	C
	ATOM	3026	CZ	PHE	234	-0.574	-68.731	105.928	1.00	18.87	B	C
20	ATOM	3027	C	PHE	234	-2.602	-62.651	107.362	1.00	20.67	B	C
	ATOM	3028	O	PHE	234	-1.936	-61.624	107.234	1.00	20.71	B	O
	ATOM	3029	N	GLN	235	-3.632	-62.740	108.194	1.00	21.02	B	N
	ATOM	3030	CA	GLN	235	-4.051	-61.614	109.020	1.00	22.09	B	C
	ATOM	3031	CB	GLN	235	-5.468	-61.845	109.548	1.00	22.57	B	C
25	ATOM	3032	CG	GLN	235	-6.481	-61.997	108.428	1.00	24.45	B	C
	ATOM	3033	CD	GLN	235	-7.898	-62.104	108.926	1.00	27.02	B	C
	ATOM	3034	OE1	GLN	235	-8.219	-62.966	109.748	1.00	27.06	B	O
	ATOM	3035	NE2	GLN	235	-8.768	-61.229	108.423	1.00	27.49	B	N
	ATOM	3036	C	GLN	235	-3.085	-61.414	110.173	1.00	21.61	B	C
30	ATOM	3037	O	GLN	235	-2.546	-62.372	110.718	1.00	21.23	B	O
	ATOM	3038	N	VAL	236	-2.876	-60.158	110.542	1.00	21.74	B	N
	ATOM	3039	CA	VAL	236	-1.957	-59.813	111.616	1.00	22.27	B	C
	ATOM	3040	CB	VAL	236	-1.915	-58.278	111.810	1.00	22.19	B	C
	ATOM	3041	CG1	VAL	236	-1.086	-57.914	113.032	1.00	22.00	B	C
35	ATOM	3042	CG2	VAL	236	-1.329	-57.628	110.562	1.00	21.53	B	C
	ATOM	3043	C	VAL	236	-2.250	-60.503	112.944	1.00	22.51	B	C
	ATOM	3044	O	VAL	236	-1.330	-60.979	113.604	1.00	22.18	B	O
	ATOM	3045	N	GLU	237	-3.521	-60.558	113.332	1.00	22.41	B	N
	ATOM	3046	CA	GLU	237	-3.928	-61.198	114.586	1.00	22.96	B	C
40	ATOM	3047	CB	GLU	237	-5.452	-61.107	114.748	1.00	25.41	B	C
	ATOM	3048	CG	GLU	237	-6.012	-61.912	115.905	1.00	29.15	B	C
	ATOM	3049	CD	GLU	237	-7.516	-61.721	116.076	1.00	31.86	B	C
	ATOM	3050	OE1	GLU	237	-8.245	-61.756	115.062	1.00	32.35	B	O
	ATOM	3051	OE2	GLU	237	-7.972	-61.545	117.227	1.00	32.72	B	O
45	ATOM	3052	C	GLU	237	-3.488	-62.659	114.628	1.00	21.89	B	C
	ATOM	3053	O	GLU	237	-2.981	-63.141	115.643	1.00	20.82	B	O
	ATOM	3054	N	PHE	238	-3.698	-63.359	113.516	1.00	20.52	B	N
	ATOM	3055	CA	PHE	238	-3.303	-64.753	113.394	1.00	19.64	B	C
	ATOM	3056	CB	PHE	238	-3.746	-65.287	112.033	1.00	18.50	B	C
50	ATOM	3057	CG	PHE	238	-3.147	-66.608	111.679	1.00	18.24	B	C
	ATOM	3058	CD1	PHE	238	-3.576	-67.771	112.303	1.00	18.18	B	C
	ATOM	3059	CD2	PHE	238	-2.133	-66.689	110.724	1.00	18.29	B	C
	ATOM	3060	CE1	PHE	238	-3.008	-69.001	111.983	1.00	18.90	B	C
	ATOM	3061	CE2	PHE	238	-1.556	-67.916	110.396	1.00	18.97	B	C
55	ATOM	3062	CZ	PHE	238	-1.994	-69.072	111.025	1.00	19.34	B	C
	ATOM	3063	C	PHE	238	-1.777	-64.831	113.526	1.00	19.52	B	C
	ATOM	3064	O	PHE	238	-1.243	-65.653	114.276	1.00	17.63	B	O
	ATOM	3065	N	LEU	239	-1.087	-63.957	112.799	1.00	19.51	B	N
	ATOM	3066	CA	LEU	239	0.372	-63.903	112.840	1.00	21.27	B	C

-222-

5	ATOM	3067	CB	LEU	239	0.881	-62.786	111.918	1.00	19.88	B	C
	ATOM	3068	CG	LEU	239	1.358	-63.090	110.485	1.00	21.98	B	C
	ATOM	3069	CD1	LEU	239	0.983	-64.488	110.062	1.00	19.74	B	C
	ATOM	3070	CD2	LEU	239	0.798	-62.046	109.521	1.00	20.05	B	C
	ATOM	3071	C	LEU	239	0.876	-63.678	114.268	1.00	21.93	B	C
10	ATOM	3072	O	LEU	239	1.819	-64.347	114.711	1.00	21.20	B	O
	ATOM	3073	N	GLU	240	0.244	-62.752	114.991	1.00	22.27	B	N
	ATOM	3074	CA	GLU	240	0.645	-62.455	116.366	1.00	24.45	B	C
	ATOM	3075	CB	GLU	240	-0.195	-61.313	116.960	1.00	26.77	B	C
	ATOM	3076	CG	GLU	240	-0.043	-59.949	116.274	1.00	30.99	B	C
15	ATOM	3077	CD	GLU	240	1.383	-59.403	116.310	1.00	34.68	B	C
	ATOM	3078	OE1	GLU	240	2.143	-59.754	117.237	1.00	37.47	B	O
	ATOM	3079	OE2	GLU	240	1.743	-58.604	115.417	1.00	36.81	B	O
	ATOM	3080	C	GLU	240	0.511	-63.689	117.254	1.00	23.48	B	C
	ATOM	3081	O	GLU	240	1.373	-63.952	118.084	1.00	23.70	B	O
20	ATOM	3082	N	LEU	241	-0.580	-64.430	117.087	1.00	22.32	B	N
	ATOM	3083	CA	LEU	241	-0.801	-65.643	117.864	1.00	21.98	B	C
	ATOM	3084	CB	LEU	241	-2.165	-66.258	117.517	1.00	23.58	B	C
	ATOM	3085	CG	LEU	241	-2.573	-67.588	118.172	1.00	25.77	B	C
	ATOM	3086	CD1	LEU	241	-2.760	-67.413	119.674	1.00	26.71	B	C
25	ATOM	3087	CD2	LEU	241	-3.869	-68.080	117.550	1.00	27.49	B	C
	ATOM	3088	C	LEU	241	0.316	-66.639	117.544	1.00	20.98	B	C
	ATOM	3089	O	LEU	241	0.858	-67.281	118.434	1.00	20.13	B	O
	ATOM	3090	N	LEU	242	0.666	-66.746	116.265	1.00	19.66	B	N
	ATOM	3091	CA	LEU	242	1.711	-67.663	115.827	1.00	19.39	B	C
30	ATOM	3092	CB	LEU	242	1.757	-67.706	114.296	1.00	17.57	B	C
	ATOM	3093	CG	LEU	242	2.800	-68.626	113.656	1.00	17.99	B	C
	ATOM	3094	CD1	LEU	242	2.679	-70.043	114.206	1.00	17.20	B	C
	ATOM	3095	CD2	LEU	242	2.593	-68.633	112.148	1.00	17.85	B	C
	ATOM	3096	C	LEU	242	3.093	-67.301	116.380	1.00	19.08	B	C
35	ATOM	3097	O	LEU	242	3.825	-68.174	116.858	1.00	18.27	B	O
	ATOM	3098	N	PHE	243	3.448	-66.020	116.322	1.00	19.06	B	N
	ATOM	3099	CA	PHE	243	4.746	-65.587	116.820	1.00	20.50	B	C
	ATOM	3100	CB	PHE	243	5.120	-64.209	116.250	1.00	20.80	B	C
	ATOM	3101	CG	PHE	243	5.719	-64.280	114.866	1.00	21.15	B	C
40	ATOM	3102	CD1	PHE	243	4.944	-64.674	113.773	1.00	21.05	B	C
	ATOM	3103	CD2	PHE	243	7.071	-64.015	114.665	1.00	20.91	B	C
	ATOM	3104	CE1	PHE	243	5.508	-64.810	112.497	1.00	21.45	B	C
	ATOM	3105	CE2	PHE	243	7.646	-64.149	113.395	1.00	21.14	B	C
	ATOM	3106	CZ	PHE	243	6.858	-64.549	112.308	1.00	21.10	B	C
45	ATOM	3107	C	PHE	243	4.821	-65.589	118.340	1.00	21.66	B	C
	ATOM	3108	O	PHE	243	5.905	-65.741	118.904	1.00	21.34	B	O
	ATOM	3109	N	HIS	244	3.673	-65.424	118.995	1.00	22.31	B	N
	ATOM	3110	CA	HIS	244	3.612	-65.456	120.448	1.00	23.28	B	C
	ATOM	3111	CB	HIS	244	2.220	-65.048	120.951	1.00	26.24	B	C
50	ATOM	3112	CG	HIS	244	1.972	-65.395	122.391	1.00	29.43	B	C
	ATOM	3113	CD2	HIS	244	2.047	-64.644	123.516	1.00	30.00	B	C
	ATOM	3114	ND1	HIS	244	1.623	-66.666	122.804	1.00	30.79	B	N
	ATOM	3115	CE1	HIS	244	1.494	-66.682	124.119	1.00	30.26	B	C
	ATOM	3116	NE2	HIS	244	1.747	-65.469	124.575	1.00	30.77	B	N
55	ATOM	3117	C	HIS	244	3.904	-66.892	120.857	1.00	21.80	B	C
	ATOM	3118	O	HIS	244	4.636	-67.133	121.809	1.00	21.67	B	O
	ATOM	3119	N	PHE	245	3.308	-67.837	120.137	1.00	19.90	B	N
	ATOM	3120	CA	PHE	245	3.529	-69.255	120.389	1.00	18.67	B	C
	ATOM	3121	CB	PHE	245	2.775	-70.104	119.356	1.00	18.04	B	C
55	ATOM	3122	CG	PHE	245	3.217	-71.540	119.316	1.00	17.45	B	C
	ATOM	3123	CD1	PHE	245	2.802	-72.439	120.294	1.00	16.43	B	C
	ATOM	3124	CD2	PHE	245	4.087	-71.985	118.321	1.00	17.18	B	C

-223-

5	ATOM	3125	CE1	PHE	245	3.244	-73.760	120.286	1.00	16.09	B	C
	ATOM	3126	CE2	PHE	245	4.539	-73.306	118.303	1.00	17.01	B	C
	ATOM	3127	CZ	PHE	245	4.117	-74.196	119.287	1.00	16.45	B	C
	ATOM	3128	C	PHE	245	5.030	-69.556	120.290	1.00	17.95	B	C
	ATOM	3129	O	PHE	245	5.600	-70.169	121.183	1.00	17.52	B	O
10	ATOM	3130	N	HIS	246	5.666	-69.115	119.206	1.00	16.92	B	N
	ATOM	3131	CA	HIS	246	7.092	-69.365	119.024	1.00	16.61	B	C
	ATOM	3132	CB	HIS	246	7.541	-68.936	117.620	1.00	15.88	B	C
	ATOM	3133	CG	HIS	246	7.208	-69.935	116.554	1.00	16.90	B	C
	ATOM	3134	CD2	HIS	246	6.248	-69.934	115.599	1.00	17.28	B	C
15	ATOM	3135	ND1	HIS	246	7.856	-71.145	116.440	1.00	16.47	B	N
	ATOM	3136	CE1	HIS	246	7.309	-71.848	115.465	1.00	16.06	B	C
	ATOM	3137	NE2	HIS	246	6.330	-71.136	114.940	1.00	15.84	B	N
	ATOM	3138	C	HIS	246	7.959	-68.704	120.095	1.00	16.14	B	C
	ATOM	3139	O	HIS	246	8.895	-69.317	120.598	1.00	16.15	B	O
20	ATOM	3140	N	GLY	247	7.666	-67.461	120.445	1.00	15.88	B	N
	ATOM	3141	CA	GLY	247	8.449	-66.813	121.488	1.00	16.58	B	C
	ATOM	3142	C	GLY	247	8.326	-67.552	122.820	1.00	17.29	B	C
	ATOM	3143	O	GLY	247	9.325	-67.849	123.474	1.00	16.50	B	O
	ATOM	3144	N	THR	248	7.097	-67.872	123.215	1.00	17.62	B	N
25	ATOM	3145	CA	THR	248	6.854	-68.569	124.473	1.00	19.52	B	C
	ATOM	3146	CB	THR	248	5.334	-68.737	124.715	1.00	20.24	B	C
	ATOM	3147	OG1	THR	248	4.694	-67.462	124.589	1.00	19.56	B	O
	ATOM	3148	CG2	THR	248	5.065	-69.288	126.110	1.00	20.09	B	C
	ATOM	3149	C	THR	248	7.536	-69.943	124.530	1.00	19.85	B	C
30	ATOM	3150	O	THR	248	8.183	-70.282	125.519	1.00	18.96	B	O
	ATOM	3151	N	LEU	249	7.392	-70.728	123.466	1.00	19.93	B	N
	ATOM	3152	CA	LEU	249	8.002	-72.047	123.412	1.00	21.38	B	C
	ATOM	3153	CB	LEU	249	7.552	-72.793	122.145	1.00	21.21	B	C
	ATOM	3154	CG	LEU	249	8.237	-74.139	121.875	1.00	19.48	B	C
35	ATOM	3155	CD1	LEU	249	7.922	-75.090	123.015	1.00	21.12	B	C
	ATOM	3156	CD2	LEU	249	7.767	-74.730	120.547	1.00	19.38	B	C
	ATOM	3157	C	LEU	249	9.526	-71.942	123.429	1.00	22.24	B	C
	ATOM	3158	O	LEU	249	10.198	-72.718	124.101	1.00	21.93	B	O
	ATOM	3159	N	ARG	250	10.058	-70.981	122.683	1.00	23.40	B	N
40	ATOM	3160	CA	ARG	250	11.499	-70.759	122.592	1.00	25.09	B	C
	ATOM	3161	CB	ARG	250	11.789	-69.621	121.613	1.00	26.51	B	C
	ATOM	3162	CG	ARG	250	12.705	-69.985	120.465	1.00	28.87	B	C
	ATOM	3163	CD	ARG	250	14.055	-70.492	120.927	1.00	28.96	B	C
	ATOM	3164	NE	ARG	250	15.002	-70.513	119.817	1.00	29.63	B	N
45	ATOM	3165	CZ	ARG	250	16.291	-70.825	119.918	1.00	31.64	B	C
	ATOM	3166	NH1	ARG	250	17.061	-70.801	118.839	1.00	32.55	B	N
	ATOM	3167	NH2	ARG	250	16.813	-71.170	121.087	1.00	32.97	B	N
	ATOM	3168	C	ARG	250	12.139	-70.411	123.932	1.00	25.34	B	C
	ATOM	3169	O	ARG	250	13.191	-70.942	124.285	1.00	24.47	B	O
50	ATOM	3170	N	LYS	251	11.508	-69.503	124.667	1.00	26.27	B	N
	ATOM	3171	CA	LYS	251	12.019	-69.071	125.963	1.00	27.02	B	C
	ATOM	3172	CB	LYS	251	11.126	-67.966	126.536	1.00	27.26	B	C
	ATOM	3173	CG	LYS	251	11.262	-66.649	125.798	1.00	30.10	B	C
	ATOM	3174	CD	LYS	251	10.253	-65.601	126.269	1.00	32.49	B	C
55	ATOM	3175	CE	LYS	251	10.377	-64.343	125.419	1.00	34.43	B	C
	ATOM	3176	NZ	LYS	251	9.361	-63.299	125.733	1.00	37.02	B	N
	ATOM	3177	C	LYS	251	12.162	-70.198	126.982	1.00	26.91	B	C
	ATOM	3178	O	LYS	251	12.861	-70.043	127.980	1.00	27.68	B	O
	ATOM	3179	N	LEU	252	11.500	-71.327	126.739	1.00	26.21	B	N
	ATOM	3180	CA	LEU	252	11.577	-72.462	127.648	1.00	25.54	B	C
	ATOM	3181	CB	LEU	252	10.405	-73.412	127.395	1.00	24.47	B	C
	ATOM	3182	CG	LEU	252	9.028	-72.881	127.809	1.00	23.94	B	C

-224-

5	ATOM	3183	CD1	LEU	252	7.948	-73.892	127.448	1.00	21.51	B	C
	ATOM	3184	CD2	LEU	252	9.026	-72.598	129.317	1.00	22.42	B	C
	ATOM	3185	C	LEU	252	12.904	-73.224	127.552	1.00	26.17	B	C
	ATOM	3186	O	LEU	252	13.200	-74.077	128.399	1.00	25.06	B	O
	ATOM	3187	N	GLN	253	13.696	-72.920	126.525	1.00	26.13	B	N
10	ATOM	3188	CA	GLN	253	14.989	-73.571	126.328	1.00	27.67	B	C
	ATOM	3189	CB	GLN	253	15.986	-73.124	127.406	1.00	29.23	B	C
	ATOM	3190	CG	GLN	253	16.176	-71.621	127.559	1.00	32.02	B	C
	ATOM	3191	CD	GLN	253	17.160	-71.282	128.673	1.00	34.60	B	C
	ATOM	3192	OE1	GLN	253	18.361	-71.531	128.552	1.00	35.64	B	O
15	ATOM	3193	NE2	GLN	253	16.651	-70.725	129.770	1.00	35.92	B	N
	ATOM	3194	C	GLN	253	14.859	-75.091	126.392	1.00	27.27	B	C
	ATOM	3195	O	GLN	253	15.553	-75.740	127.170	1.00	27.62	B	O
	ATOM	3196	N	LEU	254	13.979	-75.659	125.578	1.00	26.25	B	N
	ATOM	3197	CA	LEU	254	13.781	-77.100	125.583	1.00	25.87	B	C
20	ATOM	3198	CB	LEU	254	12.541	-77.484	124.763	1.00	23.25	B	C
	ATOM	3199	CG	LEU	254	11.166	-76.992	125.211	1.00	21.49	B	C
	ATOM	3200	CD1	LEU	254	10.100	-77.661	124.364	1.00	20.44	B	C
	ATOM	3201	CD2	LEU	254	10.957	-77.324	126.672	1.00	20.62	B	C
	ATOM	3202	C	LEU	254	14.970	-77.869	125.029	1.00	26.84	B	C
25	ATOM	3203	O	LEU	254	15.716	-77.373	124.187	1.00	26.79	B	O
	ATOM	3204	N	GLN	255	15.135	-79.090	125.514	1.00	27.67	B	N
	ATOM	3205	CA	GLN	255	16.191	-79.964	125.037	1.00	29.47	B	C
	ATOM	3206	CB	GLN	255	16.725	-80.802	126.203	1.00	31.78	B	C
	ATOM	3207	CG	GLN	255	17.397	-79.913	127.263	1.00	36.11	B	C
30	ATOM	3208	CD	GLN	255	17.854	-80.644	128.518	1.00	38.94	B	C
	ATOM	3209	OE1	GLN	255	18.321	-80.015	129.476	1.00	40.55	B	O
	ATOM	3210	NE2	GLN	255	17.729	-81.966	128.523	1.00	39.29	B	N
	ATOM	3211	C	GLN	255	15.520	-80.811	123.952	1.00	28.90	B	C
	ATOM	3212	O	GLN	255	14.296	-80.956	123.954	1.00	28.37	B	O
35	ATOM	3213	N	GLU	256	16.297	-81.341	123.013	1.00	28.82	B	N
	ATOM	3214	CA	GLU	256	15.719	-82.122	121.922	1.00	29.56	B	C
	ATOM	3215	CB	GLU	256	16.806	-82.818	121.102	1.00	30.58	B	C
	ATOM	3216	CG	GLU	256	17.589	-81.895	120.205	1.00	32.90	B	C
	ATOM	3217	CD	GLU	256	18.390	-82.652	119.163	1.00	34.07	B	C
40	ATOM	3218	OE1	GLU	256	19.015	-83.674	119.514	1.00	35.05	B	O
	ATOM	3219	OE2	GLU	256	18.402	-82.219	117.995	1.00	35.39	B	O
	ATOM	3220	C	GLU	256	14.658	-83.154	122.274	1.00	29.06	B	C
	ATOM	3221	O	GLU	256	13.587	-83.160	121.677	1.00	29.72	B	O
	ATOM	3222	N	PRO	257	14.935	-84.051	123.232	1.00	28.49	B	N
45	ATOM	3223	CD	PRO	257	16.157	-84.286	124.019	1.00	28.69	B	C
	ATOM	3224	CA	PRO	257	13.901	-85.042	123.552	1.00	27.78	B	C
	ATOM	3225	CB	PRO	257	14.551	-85.894	124.647	1.00	28.06	B	C
	ATOM	3226	CG	PRO	257	15.624	-85.012	125.201	1.00	29.28	B	C
	ATOM	3227	C	PRO	257	12.557	-84.447	123.958	1.00	26.26	B	C
50	ATOM	3228	O	PRO	257	11.519	-85.088	123.806	1.00	25.48	B	O
	ATOM	3229	N	GLU	258	12.571	-83.220	124.466	1.00	25.25	B	N
	ATOM	3230	CA	GLU	258	11.330	-82.562	124.851	1.00	24.25	B	C
	ATOM	3231	CB	GLU	258	11.631	-81.427	125.831	1.00	24.97	B	C
	ATOM	3232	CG	GLU	258	12.345	-81.953	127.069	1.00	25.66	B	C
55	ATOM	3233	CD	GLU	258	12.787	-80.879	128.029	1.00	25.87	B	C
	ATOM	3234	OE1	GLU	258	13.412	-79.897	127.581	1.00	25.45	B	O
	ATOM	3235	OE2	GLU	258	12.521	-81.034	129.240	1.00	25.58	B	O
	ATOM	3236	C	GLU	258	10.634	-82.060	123.587	1.00	23.02	B	C
	ATOM	3237	O	GLU	258	9.423	-82.212	123.442	1.00	22.77	B	O
	ATOM	3238	N	TYR	259	11.401	-81.481	122.666	1.00	21.21	B	N
	ATOM	3239	CA	TYR	259	10.846	-81.004	121.399	1.00	20.28	B	C
	ATOM	3240	CB	TYR	259	11.939	-80.378	120.527	1.00	18.72	B	C

-225-

	ATOM	3241	CG	TYR	259	12.113	-78.882	120.686	1.00	18.66	B	C
	ATOM	3242	CD1	TYR	259	11.074	-77.997	120.378	1.00	18.05	B	C
	ATOM	3243	CE1	TYR	259	11.251	-76.616	120.487	1.00	17.04	B	C
5	ATOM	3244	CD2	TYR	259	13.328	-78.346	121.110	1.00	16.85	B	C
	ATOM	3245	CE2	TYR	259	13.515	-76.976	121.220	1.00	15.76	B	C
	ATOM	3246	CZ	TYR	259	12.479	-76.114	120.905	1.00	17.18	B	C
	ATOM	3247	OH	TYR	259	12.692	-74.750	120.968	1.00	16.41	B	O
	ATOM	3248	C	TYR	259	10.253	-82.195	120.646	1.00	20.33	B	C
10	ATOM	3249	O	TYR	259	9.143	-82.123	120.101	1.00	19.27	B	O
	ATOM	3250	N	VAL	260	11.009	-83.289	120.618	1.00	20.16	B	N
	ATOM	3251	CA	VAL	260	10.588	-84.498	119.930	1.00	22.13	B	C
	ATOM	3252	CB	VAL	260	11.730	-85.535	119.921	1.00	24.17	B	C
	ATOM	3253	CG1	VAL	260	11.205	-86.882	119.500	1.00	24.73	B	C
	ATOM	3254	CG2	VAL	260	12.822	-85.088	118.949	1.00	25.03	B	C
15	ATOM	3255	C	VAL	260	9.324	-85.119	120.530	1.00	21.91	B	C
	ATOM	3256	O	VAL	260	8.428	-85.541	119.796	1.00	21.90	B	O
	ATOM	3257	N	LEU	261	9.249	-85.181	121.855	1.00	21.23	B	N
	ATOM	3258	CA	LEU	261	8.074	-85.746	122.516	1.00	22.69	B	C
20	ATOM	3259	CB	LEU	261	8.334	-85.912	124.019	1.00	22.40	B	C
	ATOM	3260	CG	LEU	261	9.193	-87.127	124.378	1.00	22.56	B	C
	ATOM	3261	CD1	LEU	261	9.560	-87.121	125.861	1.00	23.42	B	C
	ATOM	3262	CD2	LEU	261	8.419	-88.390	124.019	1.00	21.06	B	C
	ATOM	3263	C	LEU	261	6.842	-84.869	122.283	1.00	22.97	B	C
25	ATOM	3264	O	LEU	261	5.721	-85.365	122.182	1.00	23.28	B	O
	ATOM	3265	N	LEU	262	7.063	-83.565	122.191	1.00	22.71	B	N
	ATOM	3266	CA	LEU	262	5.992	-82.611	121.950	1.00	23.51	B	C
	ATOM	3267	CB	LEU	262	6.568	-81.194	122.027	1.00	24.71	B	C
	ATOM	3268	CG	LEU	262	5.647	-80.042	122.429	1.00	27.53	B	C
30	ATOM	3269	CD1	LEU	262	5.105	-80.278	123.839	1.00	27.55	B	C
	ATOM	3270	CD2	LEU	262	6.427	-78.733	122.369	1.00	27.91	B	C
	ATOM	3271	C	LEU	262	5.396	-82.889	120.555	1.00	23.38	B	C
	ATOM	3272	O	LEU	262	4.170	-82.918	120.376	1.00	22.75	B	O
	ATOM	3273	N	ALA	263	6.270	-83.100	119.572	1.00	22.06	B	N
35	ATOM	3274	CA	ALA	263	5.834	-83.399	118.215	1.00	22.18	B	C
	ATOM	3275	CB	ALA	263	7.036	-83.499	117.285	1.00	20.60	B	C
	ATOM	3276	C	ALA	263	5.071	-84.722	118.231	1.00	22.24	B	C
	ATOM	3277	O	ALA	263	4.030	-84.852	117.585	1.00	22.01	B	O
	ATOM	3278	N	ALA	264	5.593	-85.702	118.965	1.00	21.91	B	N
40	ATOM	3279	CA	ALA	264	4.938	-87.005	119.073	1.00	22.99	B	C
	ATOM	3280	CB	ALA	264	5.795	-87.961	119.905	1.00	23.25	B	C
	ATOM	3281	C	ALA	264	3.551	-86.861	119.707	1.00	23.31	B	C
	ATOM	3282	O	ALA	264	2.602	-87.538	119.307	1.00	23.47	B	O
	ATOM	3283	N	MET	265	3.434	-85.987	120.702	1.00	23.39	B	N
45	ATOM	3284	CA	MET	265	2.152	-85.774	121.359	1.00	24.89	B	C
	ATOM	3285	CB	MET	265	2.326	-84.923	122.617	1.00	26.27	B	C
	ATOM	3286	CG	MET	265	2.960	-85.692	123.761	1.00	28.18	B	C
	ATOM	3287	SD	MET	265	3.160	-84.705	125.239	1.00	30.04	B	S
	ATOM	3288	CE	MET	265	1.493	-84.692	125.842	1.00	28.25	B	C
50	ATOM	3289	C	MET	265	1.152	-85.126	120.415	1.00	24.62	B	C
	ATOM	3290	O	MET	265	-0.040	-85.407	120.487	1.00	24.02	B	O
	ATOM	3291	N	ALA	266	1.638	-84.258	119.531	1.00	24.92	B	N
	ATOM	3292	CA	ALA	266	0.771	-83.608	118.550	1.00	25.19	B	C
	ATOM	3293	CB	ALA	266	1.531	-82.476	117.835	1.00	23.17	B	C
55	ATOM	3294	C	ALA	266	0.325	-84.668	117.532	1.00	25.75	B	C
	ATOM	3295	O	ALA	266	-0.847	-84.734	117.156	1.00	25.62	B	O
	ATOM	3296	N	LEU	267	1.278	-85.491	117.092	1.00	25.83	B	N
	ATOM	3297	CA	LEU	267	1.022	-86.554	116.123	1.00	26.87	B	C
	ATOM	3298	CB	LEU	267	2.296	-87.377	115.891	1.00	26.43	B	C

-226-

5	ATOM	3299	CG	LEU	267	2.542	-88.069	114.541	1.00	27.28	B	C
	ATOM	3300	CD1	LEU	267	3.607	-89.134	114.721	1.00	26.00	B	C
	ATOM	3301	CD2	LEU	267	1.281	-88.692	113.999	1.00	27.86	B	C
	ATOM	3302	C	LEU	267	-0.081	-87.505	116.596	1.00	27.40	B	C
	ATOM	3303	O	LEU	267	-1.059	-87.741	115.883	1.00	27.12	B	O
10	ATOM	3304	N	PHE	268	0.084	-88.047	117.799	1.00	28.25	B	N
	ATOM	3305	CA	PHE	268	-0.876	-89.006	118.341	1.00	30.10	B	C
	ATOM	3306	CB	PHE	268	-0.145	-90.017	119.233	1.00	28.85	B	C
	ATOM	3307	CG	PHE	268	0.824	-90.889	118.483	1.00	28.85	B	C
	ATOM	3308	CD1	PHE	268	2.184	-90.857	118.777	1.00	28.83	B	C
15	ATOM	3309	CD2	PHE	268	0.380	-91.709	117.451	1.00	28.35	B	C
	ATOM	3310	CE1	PHE	268	3.091	-91.629	118.047	1.00	30.17	B	C
	ATOM	3311	CE2	PHE	268	1.276	-92.486	116.713	1.00	29.06	B	C
	ATOM	3312	CZ	PHE	268	2.635	-92.447	117.008	1.00	28.98	B	C
	ATOM	3313	C	PHE	268	-2.078	-88.427	119.084	1.00	31.65	B	C
20	ATOM	3314	O	PHE	268	-2.299	-88.727	120.255	1.00	31.36	B	O
	ATOM	3315	N	SER	269	-2.858	-87.611	118.386	1.00	34.17	B	N
	ATOM	3316	CA	SER	269	-4.054	-87.004	118.961	1.00	36.81	B	C
	ATOM	3317	CB	SER	269	-4.240	-85.581	118.435	1.00	36.42	B	C
	ATOM	3318	OG	SER	269	-3.138	-84.767	118.789	1.00	37.62	B	O
25	ATOM	3319	C	SER	269	-5.260	-87.854	118.566	1.00	38.85	B	C
	ATOM	3320	O	SER	269	-5.567	-87.996	117.380	1.00	38.42	B	O
	ATOM	3321	N	PRO	270	-5.959	-88.428	119.561	1.00	40.51	B	N
	ATOM	3322	CD	PRO	270	-5.665	-88.310	121.002	1.00	40.82	B	C
	ATOM	3323	CA	PRO	270	-7.138	-89.275	119.336	1.00	41.97	B	C
30	ATOM	3324	CB	PRO	270	-7.342	-89.938	120.695	1.00	41.86	B	C
	ATOM	3325	CG	PRO	270	-6.941	-88.839	121.643	1.00	41.56	B	C
	ATOM	3326	C	PRO	270	-8.391	-88.532	118.871	1.00	43.29	B	C
	ATOM	3327	O	PRO	270	-9.311	-89.141	118.325	1.00	43.76	B	O
	ATOM	3328	N	ASP	271	-8.429	-87.222	119.088	1.00	44.33	B	N
35	ATOM	3329	CA	ASP	271	-9.585	-86.424	118.696	1.00	45.68	B	C
	ATOM	3330	CB	ASP	271	-9.881	-85.370	119.774	1.00	46.97	B	C
	ATOM	3331	CG	ASP	271	-8.764	-84.350	119.928	1.00	48.52	B	C
	ATOM	3332	OD1	ASP	271	-7.578	-84.724	119.795	1.00	49.44	B	O
	ATOM	3333	OD2	ASP	271	-9.075	-83.168	120.202	1.00	49.05	B	O
40	ATOM	3334	C	ASP	271	-9.389	-85.765	117.334	1.00	45.97	B	C
	ATOM	3335	O	ASP	271	-9.848	-84.651	117.089	1.00	45.91	B	O
	ATOM	3336	N	ARG	272	-8.707	-86.476	116.444	1.00	45.79	B	N
	ATOM	3337	CA	ARG	272	-8.448	-85.977	115.108	1.00	45.77	B	C
	ATOM	3338	CB	ARG	272	-7.094	-86.489	114.612	1.00	44.26	B	C
45	ATOM	3339	CG	ARG	272	-6.217	-85.425	113.998	1.00	41.89	B	C
	ATOM	3340	CD	ARG	272	-5.168	-84.917	114.976	1.00	39.65	B	C
	ATOM	3341	NE	ARG	272	-5.198	-83.463	115.076	1.00	38.37	B	N
	ATOM	3342	CZ	ARG	272	-4.192	-82.703	115.503	1.00	37.88	B	C
	ATOM	3343	NH1	ARG	272	-3.037	-83.239	115.876	1.00	37.41	B	N
50	ATOM	3344	NH2	ARG	272	-4.351	-81.392	115.565	1.00	36.36	B	N
	ATOM	3345	C	ARG	272	-9.552	-86.476	114.182	1.00	46.79	B	C
	ATOM	3346	O	ARG	272	-9.843	-87.671	114.135	1.00	46.53	B	O
	ATOM	3347	N	PRO	273	-10.185	-85.564	113.432	1.00	47.81	B	N
	ATOM	3348	CD	PRO	273	-9.883	-84.133	113.255	1.00	48.15	B	C
55	ATOM	3349	CA	PRO	273	-11.252	-85.992	112.525	1.00	48.97	B	C
	ATOM	3350	CB	PRO	273	-11.603	-84.704	111.772	1.00	48.79	B	C
	ATOM	3351	CG	PRO	273	-10.332	-83.897	111.838	1.00	48.65	B	C
	ATOM	3352	C	PRO	273	-10.813	-87.125	111.594	1.00	49.83	B	C
	ATOM	3353	O	PRO	273	-9.809	-87.009	110.890	1.00	49.98	B	O
	ATOM	3354	N	GLY	274	-11.566	-88.223	111.615	1.00	50.41	B	N
	ATOM	3355	CA	GLY	274	-11.257	-89.363	110.769	1.00	51.30	B	C
	ATOM	3356	C	GLY	274	-10.578	-90.544	111.443	1.00	52.28	B	C

-227-

	ATOM	3357	O	GLY	274	-10.367	-91.577	110.806	1.00	52.21	B	O
	ATOM	3358	N	VAL	275	-10.234	-90.412	112.722	1.00	53.24	B	N
	ATOM	3359	CA	VAL	275	-9.569	-91.500	113.437	1.00	54.29	B	C
5	ATOM	3360	CB	VAL	275	-8.796	-90.984	114.678	1.00	54.20	B	C
	ATOM	3361	CG1	VAL	275	-7.667	-90.054	114.242	1.00	54.52	B	C
	ATOM	3362	CG2	VAL	275	-9.742	-90.268	115.621	1.00	54.74	B	C
	ATOM	3363	C	VAL	275	-10.525	-92.604	113.886	1.00	54.76	B	C
	ATOM	3364	O	VAL	275	-11.548	-92.348	114.524	1.00	54.98	B	O
10	ATOM	3365	N	THR	276	-10.170	-93.835	113.539	1.00	55.29	B	N
	ATOM	3366	CA	THR	276	-10.951	-95.014	113.883	1.00	55.88	B	C
	ATOM	3367	CB	THR	276	-10.716	-96.152	112.865	1.00	55.89	B	C
	ATOM	3368	OG1	THR	276	-10.935	-95.665	111.536	1.00	55.88	B	O
	ATOM	3369	CG2	THR	276	-11.661	-97.315	113.140	1.00	56.57	B	C
15	ATOM	3370	C	THR	276	-10.538	-95.527	115.260	1.00	56.10	B	C
	ATOM	3371	O	THR	276	-11.356	-95.625	116.173	1.00	56.37	B	O
	ATOM	3372	N	GLN	277	-9.254	-95.848	115.387	1.00	56.20	B	N
	ATOM	3373	CA	GLN	277	-8.673	-96.374	116.618	1.00	56.61	B	C
	ATOM	3374	CB	GLN	277	-7.334	-97.051	116.292	1.00	57.07	B	C
20	ATOM	3375	CG	GLN	277	-7.407	-98.557	116.026	1.00	58.02	B	C
	ATOM	3376	CD	GLN	277	-8.628	-98.975	115.228	1.00	58.03	B	C
	ATOM	3377	OE1	GLN	277	-8.868	-98.484	114.126	1.00	59.02	B	O
	ATOM	3378	NE2	GLN	277	-9.406	-99.895	115.784	1.00	58.06	B	N
	ATOM	3379	C	GLN	277	-8.459	-95.320	117.707	1.00	56.48	B	C
25	ATOM	3380	O	GLN	277	-7.325	-95.088	118.130	1.00	56.27	B	O
	ATOM	3381	N	ARG	278	-9.542	-94.700	118.172	1.00	56.44	B	N
	ATOM	3382	CA	ARG	278	-9.443	-93.672	119.205	1.00	56.32	B	C
	ATOM	3383	CB	ARG	278	-10.828	-93.134	119.574	1.00	57.69	B	C
	ATOM	3384	CG	ARG	278	-11.466	-92.272	118.495	1.00	59.91	B	C
30	ATOM	3385	CD	ARG	278	-12.365	-91.203	119.105	1.00	62.28	B	C
	ATOM	3386	NE	ARG	278	-11.597	-90.261	119.921	1.00	64.42	B	N
	ATOM	3387	CZ	ARG	278	-12.106	-89.193	120.534	1.00	65.26	B	C
	ATOM	3388	NH1	ARG	278	-13.401	-88.910	120.436	1.00	65.68	B	N
	ATOM	3389	NH2	ARG	278	-11.312	-88.400	121.243	1.00	65.69	B	N
35	ATOM	3390	C	ARG	278	-8.729	-94.136	120.467	1.00	55.50	B	C
	ATOM	3391	O	ARG	278	-7.716	-93.559	120.850	1.00	55.10	B	O
	ATOM	3392	N	ASP	279	-9.252	-95.172	121.116	1.00	54.66	B	N
	ATOM	3393	CA	ASP	279	-8.631	-95.682	122.337	1.00	54.08	B	C
	ATOM	3394	CB	ASP	279	-9.395	-96.901	122.869	1.00	55.13	B	C
40	ATOM	3395	CG	ASP	279	-10.838	-96.583	123.205	1.00	56.06	B	C
	ATOM	3396	OD1	ASP	279	-11.079	-95.570	123.898	1.00	56.83	B	O
	ATOM	3397	OD2	ASP	279	-11.730	-97.349	122.782	1.00	56.30	B	O
	ATOM	3398	C	ASP	279	-7.175	-96.067	122.102	1.00	53.02	B	C
	ATOM	3399	O	ASP	279	-6.306	-95.790	122.928	1.00	52.50	B	O
45	ATOM	3400	N	GLU	280	-6.921	-96.714	120.971	1.00	52.25	B	N
	ATOM	3401	CA	GLU	280	-5.580	-97.151	120.607	1.00	51.45	B	C
	ATOM	3402	CB	GLU	280	-5.605	-97.809	119.221	1.00	53.05	B	C
	ATOM	3403	CG	GLU	280	-6.329	-99.165	119.136	1.00	55.94	B	C
	ATOM	3404	CD	GLU	280	-7.831	-99.090	119.421	1.00	57.54	B	C
50	ATOM	3405	OE1	GLU	280	-8.530	-98.264	118.794	1.00	57.75	B	O
	ATOM	3406	OE2	GLU	280	-8.315	-99.868	120.271	1.00	59.21	B	O
	ATOM	3407	C	GLU	280	-4.599	-95.974	120.605	1.00	49.94	B	C
	ATOM	3408	O	GLU	280	-3.528	-96.036	121.211	1.00	49.12	B	O
	ATOM	3409	N	ILE	281	-4.978	-94.902	119.919	1.00	48.25	B	N
55	ATOM	3410	CA	ILE	281	-4.146	-93.712	119.827	1.00	46.84	B	C
	ATOM	3411	CB	ILE	281	-4.620	-92.812	118.660	1.00	46.36	B	C
	ATOM	3412	CG2	ILE	281	-3.836	-91.504	118.645	1.00	45.98	B	C
	ATOM	3413	CG1	ILE	281	-4.449	-93.566	117.334	1.00	45.32	B	C
	ATOM	3414	CD1	ILE	281	-4.913	-92.803	116.116	1.00	45.69	B	C

-228-

5	ATOM	3415	C	ILE	281	-4.133	-92.912	121.132	1.00	46.37	B	C
	ATOM	3416	O	ILE	281	-3.146	-92.248	121.445	1.00	46.02	B	O
	ATOM	3417	N	ASP	282	-5.223	-92.986	121.894	1.00	46.17	B	N
	ATOM	3418	CA	ASP	282	-5.324	-92.272	123.166	1.00	45.94	B	C
	ATOM	3419	CB	ASP	282	-6.719	-92.451	123.777	1.00	46.56	B	C
10	ATOM	3420	CG	ASP	282	-6.918	-91.618	125.038	1.00	48.23	B	C
	ATOM	3421	OD1	ASP	282	-6.723	-90.381	124.981	1.00	48.42	B	O
	ATOM	3422	OD2	ASP	282	-7.275	-92.197	126.089	1.00	48.95	B	O
	ATOM	3423	C	ASP	282	-4.261	-92.780	124.134	1.00	45.01	B	C
	ATOM	3424	O	ASP	282	-3.659	-92.000	124.864	1.00	45.05	B	O
15	ATOM	3425	N	GLN	283	-4.028	-94.088	124.129	1.00	44.59	B	N
	ATOM	3426	CA	GLN	283	-3.018	-94.696	124.994	1.00	43.67	B	C
	ATOM	3427	CB	GLN	283	-3.177	-96.220	124.999	1.00	45.52	B	C
	ATOM	3428	CG	GLN	283	-4.438	-96.701	125.705	1.00	48.81	B	C
	ATOM	3429	CD	GLN	283	-4.612	-98.206	125.633	1.00	51.03	B	C
20	ATOM	3430	OE1	GLN	283	-3.712	-98.967	126.000	1.00	52.12	B	O
	ATOM	3431	NE2	GLN	283	-5.778	-98.646	125.162	1.00	51.60	B	N
	ATOM	3432	C	GLN	283	-1.601	-94.328	124.550	1.00	41.87	B	C
	ATOM	3433	O	GLN	283	-0.710	-94.154	125.376	1.00	40.63	B	O
	ATOM	3434	N	LEU	284	-1.395	-94.218	123.243	1.00	40.30	B	N
25	ATOM	3435	CA	LEU	284	-0.085	-93.856	122.718	1.00	39.29	B	C
	ATOM	3436	CB	LEU	284	-0.092	-93.918	121.185	1.00	39.37	B	C
	ATOM	3437	CG	LEU	284	0.335	-95.249	120.550	1.00	39.93	B	C
	ATOM	3438	CD1	LEU	284	-0.345	-96.415	121.249	1.00	40.63	B	C
	ATOM	3439	CD2	LEU	284	-0.001	-95.239	119.067	1.00	38.88	B	C
30	ATOM	3440	C	LEU	284	0.303	-92.456	123.188	1.00	37.95	B	C
	ATOM	3441	O	LEU	284	1.425	-92.231	123.638	1.00	37.80	B	O
	ATOM	3442	N	GLN	285	-0.625	-91.514	123.092	1.00	36.96	B	N
	ATOM	3443	CA	GLN	285	-0.326	-90.164	123.529	1.00	36.82	B	C
	ATOM	3444	CB	GLN	285	-1.483	-89.215	123.239	1.00	37.92	B	C
35	ATOM	3445	CG	GLN	285	-1.222	-87.811	123.761	1.00	39.28	B	C
	ATOM	3446	CD	GLN	285	-2.277	-86.841	123.334	1.00	40.09	B	C
	ATOM	3447	OE1	GLN	285	-2.244	-86.323	122.218	1.00	41.73	B	O
	ATOM	3448	NE2	GLN	285	-3.241	-86.594	124.211	1.00	40.92	B	N
	ATOM	3449	C	GLN	285	-0.013	-90.141	125.016	1.00	36.21	B	C
40	ATOM	3450	O	GLN	285	0.902	-89.438	125.436	1.00	34.84	B	O
	ATOM	3451	N	GLU	286	-0.768	-90.904	125.810	1.00	35.91	B	N
	ATOM	3452	CA	GLU	286	-0.525	-90.958	127.249	1.00	36.06	B	C
	ATOM	3453	CB	GLU	286	-1.528	-91.884	127.937	1.00	38.35	B	C
	ATOM	3454	CG	GLU	286	-1.323	-91.998	129.446	1.00	42.49	B	C
45	ATOM	3455	CD	GLU	286	-1.209	-90.639	130.124	1.00	44.67	B	C
	ATOM	3456	OE1	GLU	286	-2.046	-89.758	129.837	1.00	46.65	B	O
	ATOM	3457	OE2	GLU	286	-0.288	-90.451	130.950	1.00	46.57	B	O
	ATOM	3458	C	GLU	286	0.895	-91.449	127.499	1.00	35.04	B	C
	ATOM	3459	O	GLU	286	1.584	-90.955	128.387	1.00	34.20	B	O
50	ATOM	3460	N	GLU	287	1.328	-92.426	126.708	1.00	34.29	B	N
	ATOM	3461	CA	GLU	287	2.678	-92.955	126.823	1.00	33.78	B	C
	ATOM	3462	CB	GLU	287	2.869	-94.123	125.851	1.00	35.48	B	C
	ATOM	3463	CG	GLU	287	4.272	-94.709	125.864	1.00	38.18	B	C
	ATOM	3464	CD	GLU	287	4.415	-95.922	124.964	1.00	40.29	B	C
55	ATOM	3465	OE1	GLU	287	5.541	-96.460	124.870	1.00	41.09	B	O
	ATOM	3466	OE2	GLU	287	3.405	-96.341	124.354	1.00	41.61	B	O
	ATOM	3467	C	GLU	287	3.671	-91.835	126.506	1.00	31.95	B	C
	ATOM	3468	O	GLU	287	4.702	-91.711	127.157	1.00	31.06	B	O
	ATOM	3469	N	MET	288	3.358	-91.023	125.499	1.00	30.97	B	N
	ATOM	3470	CA	MET	288	4.227	-89.908	125.129	1.00	30.15	B	C
	ATOM	3471	CB	MET	288	3.695	-89.179	123.883	1.00	30.43	B	C
	ATOM	3472	CG	MET	288	3.437	-90.031	122.645	1.00	30.98	B	C

-229-

5	ATOM	3473	SD	MET	288	4.901	-90.867	122.003	1.00	33.03	B	S
	ATOM	3474	CE	MET	288	4.384	-92.607	122.202	1.00	32.43	B	C
	ATOM	3475	C	MET	288	4.251	-88.919	126.300	1.00	28.89	B	C
	ATOM	3476	O	MET	288	5.310	-88.489	126.751	1.00	28.59	B	O
	ATOM	3477	N	ALA	289	3.065	-88.568	126.786	1.00	28.24	B	N
10	ATOM	3478	CA	ALA	289	2.920	-87.622	127.887	1.00	28.40	B	C
	ATOM	3479	CB	ALA	289	1.441	-87.415	128.195	1.00	27.31	B	C
	ATOM	3480	C	ALA	289	3.674	-88.059	129.146	1.00	28.77	B	C
	ATOM	3481	O	ALA	289	4.356	-87.248	129.777	1.00	28.99	B	O
	ATOM	3482	N	LEU	290	3.555	-89.333	129.511	1.00	29.19	B	N
15	ATOM	3483	CA	LEU	290	4.248	-89.850	130.688	1.00	29.74	B	C
	ATOM	3484	CB	LEU	290	3.786	-91.271	131.019	1.00	31.00	B	C
	ATOM	3485	CG	LEU	290	2.366	-91.417	131.574	1.00	33.11	B	C
	ATOM	3486	CD1	LEU	290	2.029	-92.895	131.750	1.00	33.94	B	C
	ATOM	3487	CD2	LEU	290	2.259	-90.677	132.908	1.00	34.21	B	C
20	ATOM	3488	C	LEU	290	5.750	-89.850	130.475	1.00	29.25	B	C
	ATOM	3489	O	LEU	290	6.510	-89.582	131.400	1.00	29.29	B	O
	ATOM	3490	N	THR	291	6.183	-90.158	129.255	1.00	28.88	B	N
	ATOM	3491	CA	THR	291	7.609	-90.169	128.959	1.00	27.56	B	C
	ATOM	3492	CB	THR	291	7.886	-90.695	127.538	1.00	27.69	B	C
25	ATOM	3493	OG1	THR	291	7.381	-92.034	127.419	1.00	27.19	B	O
	ATOM	3494	CG2	THR	291	9.385	-90.688	127.248	1.00	25.40	B	C
	ATOM	3495	C	THR	291	8.159	-88.753	129.090	1.00	27.38	B	C
	ATOM	3496	O	THR	291	9.243	-88.554	129.637	1.00	26.70	B	O
	ATOM	3497	N	LEU	292	7.410	-87.772	128.586	1.00	26.91	B	N
30	ATOM	3498	CA	LEU	292	7.829	-86.378	128.681	1.00	27.05	B	C
	ATOM	3499	CB	LEU	292	6.847	-85.471	127.928	1.00	25.96	B	C
	ATOM	3500	CG	LEU	292	7.139	-83.963	127.939	1.00	25.61	B	C
	ATOM	3501	CD1	LEU	292	8.590	-83.708	127.580	1.00	23.77	B	C
	ATOM	3502	CD2	LEU	292	6.202	-83.244	126.966	1.00	24.54	B	C
35	ATOM	3503	C	LEU	292	7.916	-85.960	130.151	1.00	27.73	B	C
	ATOM	3504	O	LEU	292	8.875	-85.308	130.554	1.00	26.74	B	O
	ATOM	3505	N	GLN	293	6.917	-86.338	130.949	1.00	29.30	B	N
	ATOM	3506	CA	GLN	293	6.915	-86.008	132.374	1.00	31.80	B	C
	ATOM	3507	CB	GLN	293	5.663	-86.564	133.059	1.00	33.01	B	C
40	ATOM	3508	CG	GLN	293	4.367	-85.871	132.675	1.00	35.44	B	C
	ATOM	3509	CD	GLN	293	3.151	-86.491	133.354	1.00	37.29	B	C
	ATOM	3510	OE1	GLN	293	3.067	-86.547	134.588	1.00	36.31	B	O
	ATOM	3511	NE2	GLN	293	2.201	-86.964	132.546	1.00	38.33	B	N
	ATOM	3512	C	GLN	293	8.155	-86.594	133.051	1.00	32.77	B	C
45	ATOM	3513	O	GLN	293	8.908	-85.875	133.707	1.00	32.11	B	O
	ATOM	3514	N	SER	294	8.356	-87.901	132.881	1.00	33.57	B	N
	ATOM	3515	CA	SER	294	9.502	-88.602	133.460	1.00	34.88	B	C
	ATOM	3516	CB	SER	294	9.550	-90.053	132.962	1.00	36.18	B	C
	ATOM	3517	OG	SER	294	8.353	-90.748	133.261	1.00	37.51	B	O
50	ATOM	3518	C	SER	294	10.808	-87.913	133.090	1.00	34.78	B	C
	ATOM	3519	O	SER	294	11.654	-87.661	133.947	1.00	34.65	B	O
	ATOM	3520	N	TYR	295	10.970	-87.613	131.805	1.00	34.99	B	N
	ATOM	3521	CA	TYR	295	12.175	-86.954	131.331	1.00	35.00	B	C
	ATOM	3522	CB	TYR	295	12.127	-86.789	129.814	1.00	34.20	B	C
55	ATOM	3523	CG	TYR	295	13.357	-86.115	129.263	1.00	33.37	B	C
	ATOM	3524	CD1	TYR	295	13.487	-84.726	129.289	1.00	32.51	B	C
	ATOM	3525	CE1	TYR	295	14.627	-84.106	128.811	1.00	32.85	B	C
	ATOM	3526	CD2	TYR	295	14.406	-86.868	128.741	1.00	33.17	B	C
	ATOM	3527	CE2	TYR	295	15.550	-86.259	128.260	1.00	32.70	B	C
	ATOM	3528	CZ	TYR	295	15.654	-84.879	128.295	1.00	33.54	B	C
	ATOM	3529	OH	TYR	295	16.779	-84.275	127.784	1.00	34.15	B	O
	ATOM	3530	C	TYR	295	12.391	-85.598	131.993	1.00	35.91	B	C

-230-

	ATOM	3531	O	TYR	295	13.510	-85.268	132.379	1.00	35.15	B	O
	ATOM	3532	N	ILE	296	11.327	-84.809	132.111	1.00	37.71	B	N
	ATOM	3533	CA	ILE	296	11.418	-83.492	132.741	1.00	40.23	B	C
5	ATOM	3534	CB	ILE	296	10.084	-82.705	132.618	1.00	39.25	B	C
	ATOM	3535	CG2	ILE	296	10.153	-81.424	133.447	1.00	38.18	B	C
	ATOM	3536	CG1	ILE	296	9.797	-82.378	131.151	1.00	38.83	B	C
	ATOM	3537	CD1	ILE	296	8.486	-81.651	130.932	1.00	38.48	B	C
	ATOM	3538	C	ILE	296	11.751	-83.639	134.227	1.00	42.98	B	C
10	ATOM	3539	O	ILE	296	12.617	-82.934	134.752	1.00	42.72	B	O
	ATOM	3540	N	LYS	297	11.050	-84.552	134.897	1.00	46.09	B	N
	ATOM	3541	CA	LYS	297	11.263	-84.799	136.317	1.00	49.98	B	C
	ATOM	3542	CB	LYS	297	10.432	-85.997	136.786	1.00	49.95	B	C
	ATOM	3543	CG	LYS	297	8.949	-85.718	136.966	1.00	50.90	B	C
15	ATOM	3544	CD	LYS	297	8.231	-86.957	137.487	1.00	51.71	B	C
	ATOM	3545	CE	LYS	297	6.745	-86.713	137.702	1.00	51.90	B	C
	ATOM	3546	NZ	LYS	297	6.063	-87.944	138.193	1.00	52.46	B	N
	ATOM	3547	C	LYS	297	12.730	-85.055	136.632	1.00	52.54	B	C
	ATOM	3548	O	LYS	297	13.306	-84.405	137.500	1.00	53.13	B	O
20	ATOM	3549	N	GLY	298	13.335	-85.998	135.919	1.00	55.39	B	N
	ATOM	3550	CA	GLY	298	14.728	-86.318	136.167	1.00	59.24	B	C
	ATOM	3551	C	GLY	298	15.742	-85.421	135.485	1.00	62.03	B	C
	ATOM	3552	O	GLY	298	16.926	-85.452	135.824	1.00	62.62	B	O
	ATOM	3553	N	GLN	299	15.293	-84.610	134.536	1.00	64.81	B	N
25	ATOM	3554	CA	GLN	299	16.210	-83.740	133.816	1.00	67.60	B	C
	ATOM	3555	CB	GLN	299	15.488	-83.006	132.688	1.00	67.76	B	C
	ATOM	3556	CG	GLN	299	16.447	-82.333	131.729	1.00	68.45	B	C
	ATOM	3557	CD	GLN	299	17.668	-83.194	131.453	1.00	68.63	B	C
	ATOM	3558	OE1	GLN	299	17.553	-84.402	131.236	1.00	68.95	B	O
30	ATOM	3559	NE2	GLN	299	18.845	-82.576	131.457	1.00	68.63	B	N
	ATOM	3560	C	GLN	299	16.927	-82.731	134.697	1.00	69.34	B	C
	ATOM	3561	O	GLN	299	16.312	-82.047	135.518	1.00	69.59	B	O
	ATOM	3562	N	GLN	300	18.240	-82.655	134.495	1.00	71.45	B	N
	ATOM	3563	CA	GLN	300	19.136	-81.764	135.221	1.00	73.26	B	C
35	ATOM	3564	CB	GLN	300	20.562	-81.917	134.676	1.00	73.69	B	C
	ATOM	3565	CG	GLN	300	21.314	-83.126	135.213	1.00	74.64	B	C
	ATOM	3566	CD	GLN	300	20.675	-84.451	134.846	1.00	75.14	B	C
	ATOM	3567	OE1	GLN	300	20.497	-84.765	133.667	1.00	75.32	B	O
	ATOM	3568	NE2	GLN	300	20.331	-85.241	135.858	1.00	75.53	B	N
40	ATOM	3569	C	GLN	300	18.720	-80.292	135.204	1.00	74.21	B	C
	ATOM	3570	O	GLN	300	17.533	-79.984	135.303	1.00	74.60	B	O
	ATOM	3571	N	ARG	301	19.703	-79.397	135.073	1.00	75.01	B	N
	ATOM	3572	CA	ARG	301	19.487	-77.948	135.086	1.00	75.30	B	C
	ATOM	3573	CB	ARG	301	18.678	-77.484	133.858	1.00	75.26	B	C
45	ATOM	3574	CG	ARG	301	17.192	-77.794	133.901	1.00	75.18	B	C
	ATOM	3575	CD	ARG	301	16.505	-77.521	132.580	1.00	75.06	B	C
	ATOM	3576	NE	ARG	301	15.450	-78.504	132.349	1.00	74.97	B	N
	ATOM	3577	CZ	ARG	301	14.658	-78.536	131.281	1.00	74.61	B	C
	ATOM	3578	NH1	ARG	301	14.779	-77.630	130.317	1.00	74.17	B	N
50	ATOM	3579	NH2	ARG	301	13.750	-79.493	131.174	1.00	74.08	B	N
	ATOM	3580	C	ARG	301	18.754	-77.615	136.384	1.00	75.55	B	C
	ATOM	3581	O	ARG	301	17.633	-78.071	136.615	1.00	75.54	B	O
	ATOM	3582	N	ARG	302	19.381	-76.816	137.240	1.00	75.70	B	N
	ATOM	3583	CA	ARG	302	18.746	-76.492	138.507	1.00	75.72	B	C
55	ATOM	3584	CB	ARG	302	19.810	-76.338	139.602	1.00	76.38	B	C
	ATOM	3585	CG	ARG	302	19.234	-76.395	141.018	1.00	77.18	B	C
	ATOM	3586	CD	ARG	302	20.152	-77.127	141.988	1.00	77.70	B	C
	ATOM	3587	NE	ARG	302	21.423	-76.437	142.207	1.00	78.27	B	N
	ATOM	3588	CZ	ARG	302	21.562	-75.290	142.868	1.00	78.26	B	C

-231-

	ATOM	3589	NH1	ARG	302	20.507	-74.674	143.391	1.00	78.27	B	N
	ATOM	3590	NH2	ARG	302	22.767	-74.760	143.016	1.00	78.37	B	N
	ATOM	3591	C	ARG	302	17.762	-75.317	138.574	1.00	75.23	B	C
5	ATOM	3592	O	ARG	302	17.499	-74.803	139.663	1.00	75.35	B	O
	ATOM	3593	N	PRO	303	17.202	-74.860	137.430	1.00	74.61	B	N
	ATOM	3594	CD	PRO	303	17.298	-75.150	135.986	1.00	74.54	B	C
	ATOM	3595	CA	PRO	303	16.273	-73.750	137.667	1.00	73.58	B	C
	ATOM	3596	CB	PRO	303	16.012	-73.215	136.261	1.00	73.72	B	C
10	ATOM	3597	CG	PRO	303	16.073	-74.451	135.427	1.00	74.08	B	C
	ATOM	3598	C	PRO	303	15.010	-74.319	138.321	1.00	72.47	B	C
	ATOM	3599	O	PRO	303	14.156	-73.579	138.807	1.00	72.47	B	O
	ATOM	3600	N	ARG	304	14.920	-75.648	138.330	1.00	71.25	B	N
	ATOM	3601	CA	ARG	304	13.796	-76.366	138.901	1.00	69.81	B	C
15	ATOM	3602	CB	ARG	304	13.947	-76.484	140.423	1.00	71.29	B	C
	ATOM	3603	CG	ARG	304	14.821	-77.652	140.877	1.00	72.92	B	C
	ATOM	3604	CD	ARG	304	14.673	-77.891	142.376	1.00	74.32	B	C
	ATOM	3605	NE	ARG	304	15.207	-79.188	142.794	1.00	75.67	B	N
	ATOM	3606	CZ	ARG	304	15.103	-79.684	144.027	1.00	76.25	B	C
20	ATOM	3607	NH1	ARG	304	14.484	-78.995	144.980	1.00	76.56	B	N
	ATOM	3608	NH2	ARG	304	15.613	-80.876	144.309	1.00	76.34	B	N
	ATOM	3609	C	ARG	304	12.464	-75.716	138.562	1.00	67.71	B	C
	ATOM	3610	O	ARG	304	11.882	-74.999	139.379	1.00	68.11	B	O
	ATOM	3611	N	ASP	305	11.989	-75.956	137.344	1.00	64.75	B	N
25	ATOM	3612	CA	ASP	305	10.708	-75.417	136.929	1.00	61.23	B	C
	ATOM	3613	CB	ASP	305	10.789	-74.800	135.534	1.00	61.94	B	C
	ATOM	3614	CG	ASP	305	9.459	-74.232	135.082	1.00	62.41	B	C
	ATOM	3615	OD1	ASP	305	8.677	-73.803	135.959	1.00	62.77	B	O
	ATOM	3616	OD2	ASP	305	9.202	-74.194	133.860	1.00	62.51	B	O
30	ATOM	3617	C	ASP	305	9.679	-76.536	136.956	1.00	58.50	B	C
	ATOM	3618	O	ASP	305	9.625	-77.382	136.059	1.00	58.07	B	O
	ATOM	3619	N	ARG	306	8.878	-76.543	138.016	1.00	54.93	B	N
	ATOM	3620	CA	ARG	306	7.840	-77.548	138.187	1.00	51.10	B	C
	ATOM	3621	CB	ARG	306	7.408	-77.604	139.651	1.00	53.42	B	C
35	ATOM	3622	CG	ARG	306	8.513	-77.985	140.611	1.00	56.34	B	C
	ATOM	3623	CD	ARG	306	8.016	-77.954	142.041	1.00	59.35	B	C
	ATOM	3624	NE	ARG	306	9.051	-78.364	142.988	1.00	61.82	B	N
	ATOM	3625	CZ	ARG	306	8.925	-78.298	144.308	1.00	62.64	B	C
	ATOM	3626	NH1	ARG	306	9.923	-78.686	145.090	1.00	62.90	B	N
40	ATOM	3627	NH2	ARG	306	7.805	-77.831	144.840	1.00	63.33	B	N
	ATOM	3628	C	ARG	306	6.644	-77.204	137.318	1.00	46.82	B	C
	ATOM	3629	O	ARG	306	5.683	-77.962	137.241	1.00	46.07	B	O
	ATOM	3630	N	PHE	307	6.714	-76.049	136.668	1.00	42.30	B	N
	ATOM	3631	CA	PHE	307	5.647	-75.583	135.807	1.00	38.22	B	C
45	ATOM	3632	CB	PHE	307	5.481	-74.068	135.962	1.00	38.24	B	C
	ATOM	3633	CG	PHE	307	5.179	-73.628	137.369	1.00	38.97	B	C
	ATOM	3634	CD1	PHE	307	6.188	-73.556	138.326	1.00	39.66	B	C
	ATOM	3635	CD2	PHE	307	3.883	-73.296	137.741	1.00	39.64	B	C
	ATOM	3636	CE1	PHE	307	5.915	-73.160	139.632	1.00	40.08	B	C
	ATOM	3637	CE2	PHE	307	3.595	-72.898	139.047	1.00	40.42	B	C
50	ATOM	3638	CZ	PHE	307	4.616	-72.830	139.993	1.00	40.42	B	C
	ATOM	3639	C	PHE	307	5.901	-75.924	134.337	1.00	35.22	B	C
	ATOM	3640	O	PHE	307	5.030	-75.731	133.494	1.00	34.63	B	O
	ATOM	3641	N	LEU	308	7.085	-76.445	134.036	1.00	32.23	B	N
55	ATOM	3642	CA	LEU	308	7.441	-76.776	132.663	1.00	29.80	B	C
	ATOM	3643	CB	LEU	308	8.818	-77.445	132.617	1.00	30.13	B	C
	ATOM	3644	CG	LEU	308	9.725	-77.108	131.427	1.00	30.71	B	C
	ATOM	3645	CD1	LEU	308	10.806	-78.172	131.314	1.00	31.09	B	C
	ATOM	3646	CD2	LEU	308	8.932	-77.041	130.142	1.00	30.29	B	C

-232-

	ATOM	3647	C	LEU	308	6.420	-77.671	131.956	1.00	27.96	B	C
	ATOM	3648	O	LEU	308	5.892	-77.296	130.911	1.00	26.38	B	O
	ATOM	3649	N	TYR	309	6.146	-78.847	132.517	1.00	26.33	B	N
5	ATOM	3650	CA	TYR	309	5.199	-79.770	131.896	1.00	26.08	B	C
	ATOM	3651	CB	TYR	309	5.037	-81.040	132.743	1.00	26.27	B	C
	ATOM	3652	CG	TYR	309	4.121	-82.074	132.109	1.00	26.57	B	C
	ATOM	3653	CD1	TYR	309	4.409	-82.611	130.855	1.00	26.55	B	C
	ATOM	3654	CE1	TYR	309	3.559	-83.533	130.249	1.00	27.76	B	C
10	ATOM	3655	CD2	TYR	309	2.955	-82.489	132.749	1.00	26.42	B	C
	ATOM	3656	CE2	TYR	309	2.092	-83.414	132.152	1.00	28.03	B	C
	ATOM	3657	CZ	TYR	309	2.404	-83.930	130.902	1.00	27.91	B	C
	ATOM	3658	OH	TYR	309	1.568	-84.847	130.312	1.00	29.13	B	O
	ATOM	3659	C	TYR	309	3.830	-79.135	131.650	1.00	25.30	B	C
15	ATOM	3660	O	TYR	309	3.261	-79.280	130.568	1.00	24.69	B	O
	ATOM	3661	N	ALA	310	3.308	-78.427	132.649	1.00	24.77	B	N
	ATOM	3662	CA	ALA	310	2.007	-77.780	132.519	1.00	23.64	B	C
	ATOM	3663	CB	ALA	310	1.628	-77.092	133.822	1.00	24.37	B	C
	ATOM	3664	C	ALA	310	2.047	-76.764	131.385	1.00	23.22	B	C
20	ATOM	3665	O	ALA	310	1.088	-76.630	130.628	1.00	22.01	B	O
	ATOM	3666	N	LYS	311	3.158	-76.043	131.276	1.00	22.47	B	N
	ATOM	3667	CA	LYS	311	3.315	-75.052	130.217	1.00	22.76	B	C
	ATOM	3668	CB	LYS	311	4.612	-74.271	130.413	1.00	23.73	B	C
	ATOM	3669	CG	LYS	311	4.563	-73.270	131.550	1.00	25.88	B	C
25	ATOM	3670	CD	LYS	311	5.880	-72.533	131.657	1.00	27.25	B	C
	ATOM	3671	CE	LYS	311	5.884	-71.568	132.820	1.00	29.50	B	C
	ATOM	3672	NZ	LYS	311	7.240	-70.971	133.000	1.00	31.45	B	N
	ATOM	3673	C	LYS	311	3.309	-75.710	128.838	1.00	20.98	B	C
	ATOM	3674	O	LYS	311	2.728	-75.185	127.900	1.00	21.17	B	O
30	ATOM	3675	N	LEU	312	3.949	-76.865	128.721	1.00	20.58	B	N
	ATOM	3676	CA	LEU	312	3.989	-77.580	127.454	1.00	20.47	B	C
	ATOM	3677	CB	LEU	312	4.968	-78.753	127.550	1.00	20.31	B	C
	ATOM	3678	CG	LEU	312	6.438	-78.356	127.715	1.00	20.12	B	C
	ATOM	3679	CD1	LEU	312	7.304	-79.599	127.750	1.00	20.29	B	C
35	ATOM	3680	CD2	LEU	312	6.853	-77.459	126.561	1.00	19.66	B	C
	ATOM	3681	C	LEU	312	2.601	-78.075	127.029	1.00	20.37	B	C
	ATOM	3682	O	LEU	312	2.274	-78.074	125.840	1.00	19.79	B	O
	ATOM	3683	N	LEU	313	1.790	-78.513	127.989	1.00	19.32	B	N
	ATOM	3684	CA	LEU	313	0.444	-78.967	127.659	1.00	19.16	B	C
40	ATOM	3685	CB	LEU	313	-0.255	-79.601	128.872	1.00	18.30	B	C
	ATOM	3686	CG	LEU	313	0.303	-80.942	129.369	1.00	19.24	B	C
	ATOM	3687	CD1	LEU	313	-0.641	-81.513	130.417	1.00	18.74	B	C
	ATOM	3688	CD2	LEU	313	0.456	-81.929	128.205	1.00	19.01	B	C
	ATOM	3689	C	LEU	313	-0.345	-77.762	127.173	1.00	18.59	B	C
45	ATOM	3690	O	LEU	313	-1.131	-77.866	126.235	1.00	18.15	B	O
	ATOM	3691	N	GLY	314	-0.123	-76.617	127.810	1.00	18.61	B	N
	ATOM	3692	CA	GLY	314	-0.803	-75.398	127.402	1.00	19.37	B	C
	ATOM	3693	C	GLY	314	-0.386	-74.990	125.999	1.00	20.32	B	C
	ATOM	3694	O	GLY	314	-1.196	-74.505	125.208	1.00	20.34	B	O
50	ATOM	3695	N	LEU	315	0.893	-75.168	125.689	1.00	20.42	B	N
	ATOM	3696	CA	LEU	315	1.394	-74.829	124.367	1.00	20.97	B	C
	ATOM	3697	CB	LEU	315	2.923	-74.823	124.368	1.00	20.14	B	C
	ATOM	3698	CG	LEU	315	3.491	-73.558	125.027	1.00	21.61	B	C
	ATOM	3699	CD1	LEU	315	4.998	-73.678	125.204	1.00	22.43	B	C
55	ATOM	3700	CD2	LEU	315	3.141	-72.341	124.174	1.00	20.16	B	C
	ATOM	3701	C	LEU	315	0.847	-75.791	123.318	1.00	20.93	B	C
	ATOM	3702	O	LEU	315	0.560	-75.380	122.200	1.00	21.86	B	O
	ATOM	3703	N	LEU	316	0.693	-77.064	123.670	1.00	20.78	B	N
	ATOM	3704	CA	LEU	316	0.140	-78.038	122.728	1.00	22.07	B	C

-233-

5	ATOM	3705	CB	LEU	316	0.122	-79.442	123.333	1.00	22.61	B	C
	ATOM	3706	CG	LEU	316	1.463	-80.171	123.415	1.00	25.13	B	C
	ATOM	3707	CD1	LEU	316	1.259	-81.562	123.994	1.00	25.21	B	C
	ATOM	3708	CD2	LEU	316	2.073	-80.266	122.021	1.00	27.32	B	C
	ATOM	3709	C	LEU	316	-1.286	-77.633	122.356	1.00	22.16	B	C
10	ATOM	3710	O	LEU	316	-1.723	-77.853	121.225	1.00	21.15	B	O
	ATOM	3711	N	ALA	317	-1.998	-77.042	123.319	1.00	22.21	B	N
	ATOM	3712	CA	ALA	317	-3.364	-76.575	123.123	1.00	22.68	B	C
	ATOM	3713	CB	ALA	317	-4.034	-76.321	124.482	1.00	22.13	B	C
	ATOM	3714	C	ALA	317	-3.380	-75.296	122.284	1.00	23.40	B	C
15	ATOM	3715	O	ALA	317	-4.256	-75.115	121.437	1.00	22.48	B	O
	ATOM	3716	N	GLU	318	-2.422	-74.404	122.527	1.00	23.64	B	N
	ATOM	3717	CA	GLU	318	-2.347	-73.164	121.763	1.00	25.42	B	C
	ATOM	3718	CB	GLU	318	-1.266	-72.242	122.325	1.00	27.16	B	C
	ATOM	3719	CG	GLU	318	-1.393	-70.797	121.859	1.00	32.13	B	C
20	ATOM	3720	CD	GLU	318	-0.190	-69.944	122.233	1.00	34.93	B	C
	ATOM	3721	OE1	GLU	318	0.321	-70.093	123.362	1.00	37.73	B	O
	ATOM	3722	OE2	GLU	318	0.239	-69.114	121.402	1.00	36.75	B	O
	ATOM	3723	C	GLU	318	-2.036	-73.490	120.298	1.00	25.14	B	C
	ATOM	3724	O	GLU	318	-2.557	-72.851	119.384	1.00	23.94	B	O
25	ATOM	3725	N	LEU	319	-1.186	-74.490	120.084	1.00	25.66	B	N
	ATOM	3726	CA	LEU	319	-0.814	-74.919	118.735	1.00	26.58	B	C
	ATOM	3727	CB	LEU	319	0.302	-75.961	118.818	1.00	27.06	B	C
	ATOM	3728	CG	LEU	319	0.981	-76.399	117.524	1.00	28.14	B	C
	ATOM	3729	CD1	LEU	319	1.450	-75.183	116.749	1.00	28.22	B	C
30	ATOM	3730	CD2	LEU	319	2.156	-77.309	117.860	1.00	28.83	B	C
	ATOM	3731	C	LEU	319	-2.047	-75.508	118.036	1.00	26.66	B	C
	ATOM	3732	O	LEU	319	-2.200	-75.420	116.815	1.00	25.59	B	O
	ATOM	3733	N	ARG	320	-2.926	-76.112	118.826	1.00	26.81	B	N
	ATOM	3734	CA	ARG	320	-4.154	-76.671	118.298	1.00	27.51	B	C
35	ATOM	3735	CB	ARG	320	-4.863	-77.471	119.388	1.00	30.21	B	C
	ATOM	3736	CG	ARG	320	-6.022	-78.298	118.892	1.00	34.14	B	C
	ATOM	3737	CD	ARG	320	-5.573	-79.252	117.808	1.00	37.44	B	C
	ATOM	3738	NE	ARG	320	-6.606	-80.233	117.500	1.00	41.15	B	N
	ATOM	3739	CZ	ARG	320	-6.749	-81.403	118.118	1.00	42.64	B	C
40	ATOM	3740	NH1	ARG	320	-5.919	-81.762	119.093	1.00	43.92	B	N
	ATOM	3741	NH2	ARG	320	-7.728	-82.222	117.755	1.00	43.56	B	N
	ATOM	3742	C	ARG	320	-5.022	-75.496	117.837	1.00	26.59	B	C
	ATOM	3743	O	ARG	320	-5.648	-75.551	116.781	1.00	26.01	B	O
	ATOM	3744	N	SER	321	-5.055	-74.430	118.635	1.00	25.46	B	N
45	ATOM	3745	CA	SER	321	-5.822	-73.235	118.283	1.00	25.37	B	C
	ATOM	3746	CB	SER	321	-5.676	-72.150	119.356	1.00	25.01	B	C
	ATOM	3747	OG	SER	321	-6.252	-72.562	120.577	1.00	28.59	B	O
	ATOM	3748	C	SER	321	-5.310	-72.681	116.964	1.00	24.05	B	C
	ATOM	3749	O	SER	321	-6.090	-72.294	116.097	1.00	23.58	B	O
50	ATOM	3750	N	ILE	322	-3.988	-72.636	116.834	1.00	23.19	B	N
	ATOM	3751	CA	ILE	322	-3.339	-72.136	115.632	1.00	23.73	B	C
	ATOM	3752	CB	ILE	322	-1.800	-72.171	115.794	1.00	24.44	B	C
	ATOM	3753	CG2	ILE	322	-1.115	-71.875	114.454	1.00	23.92	B	C
	ATOM	3754	CG1	ILE	322	-1.381	-71.170	116.878	1.00	24.48	B	C
55	ATOM	3755	CD1	ILE	322	0.068	-71.277	117.301	1.00	25.71	B	C
	ATOM	3756	C	ILE	322	-3.759	-72.963	114.418	1.00	23.91	B	C
	ATOM	3757	O	ILE	322	-4.004	-72.418	113.342	1.00	23.08	B	O
	ATOM	3758	N	ASN	323	-3.853	-74.276	114.601	1.00	24.23	B	N
	ATOM	3759	CA	ASN	323	-4.258	-75.172	113.525	1.00	26.82	B	C
	ATOM	3760	CB	ASN	323	-4.286	-76.617	114.033	1.00	29.48	B	C
	ATOM	3761	CG	ASN	323	-4.045	-77.635	112.929	1.00	32.74	B	C
	ATOM	3762	OD1	ASN	323	-4.426	-78.796	113.058	1.00	32.81	B	O

-234-

5	ATOM	3763	ND2	ASN	323	-3.386	-77.208	111.846	1.00	34.14	B	N
	ATOM	3764	C	ASN	323	-5.652	-74.764	113.033	1.00	27.38	B	C
	ATOM	3765	O	ASN	323	-5.856	-74.546	111.840	1.00	26.41	B	O
	ATOM	3766	N	GLU	324	-6.607	-74.656	113.959	1.00	27.46	B	N
	ATOM	3767	CA	GLU	324	-7.963	-74.246	113.612	1.00	28.72	B	C
10	ATOM	3768	CB	GLU	324	-8.867	-74.253	114.852	1.00	30.37	B	C
	ATOM	3769	CG	GLU	324	-8.979	-75.615	115.533	1.00	34.56	B	C
	ATOM	3770	CD	GLU	324	-9.872	-75.585	116.766	1.00	37.51	B	C
	ATOM	3771	OE1	GLU	324	-9.717	-74.660	117.598	1.00	38.60	B	O
	ATOM	3772	OE2	GLU	324	-10.723	-76.492	116.909	1.00	39.78	B	O
15	ATOM	3773	C	GLU	324	-7.959	-72.846	112.992	1.00	27.55	B	C
	ATOM	3774	O	GLU	324	-8.712	-72.574	112.062	1.00	28.12	B	O
	ATOM	3775	N	ALA	325	-7.118	-71.959	113.512	1.00	25.61	B	N
	ATOM	3776	CA	ALA	325	-7.032	-70.607	112.985	1.00	24.75	B	C
	ATOM	3777	CB	ALA	325	-6.102	-69.763	113.852	1.00	25.33	B	C
20	ATOM	3778	C	ALA	325	-6.537	-70.642	111.539	1.00	24.31	B	C
	ATOM	3779	O	ALA	325	-6.905	-69.793	110.726	1.00	24.70	B	O
	ATOM	3780	N	TYR	326	-5.688	-71.613	111.223	1.00	23.49	B	N
	ATOM	3781	CA	TYR	326	-5.192	-71.763	109.861	1.00	23.05	B	C
	ATOM	3782	CB	TYR	326	-4.233	-72.958	109.756	1.00	21.78	B	C
25	ATOM	3783	CG	TYR	326	-2.770	-72.576	109.741	1.00	20.85	B	C
	ATOM	3784	CD1	TYR	326	-2.232	-71.844	108.683	1.00	20.27	B	C
	ATOM	3785	CE1	TYR	326	-0.886	-71.492	108.664	1.00	19.55	B	C
	ATOM	3786	CD2	TYR	326	-1.921	-72.945	110.782	1.00	20.45	B	C
	ATOM	3787	CE2	TYR	326	-0.575	-72.596	110.771	1.00	19.56	B	C
30	ATOM	3788	CZ	TYR	326	-0.070	-71.872	109.711	1.00	19.09	B	C
	ATOM	3789	OH	TYR	326	1.250	-71.527	109.701	1.00	17.47	B	O
	ATOM	3790	C	TYR	326	-6.399	-72.001	108.961	1.00	23.60	B	C
	ATOM	3791	O	TYR	326	-6.502	-71.422	107.876	1.00	23.00	B	O
	ATOM	3792	N	GLY	327	-7.304	-72.862	109.425	1.00	23.42	B	N
35	ATOM	3793	CA	GLY	327	-8.503	-73.174	108.669	1.00	24.68	B	C
	ATOM	3794	C	GLY	327	-9.318	-71.936	108.354	1.00	26.46	B	C
	ATOM	3795	O	GLY	327	-9.790	-71.773	107.234	1.00	25.91	B	O
	ATOM	3796	N	TYR	328	-9.491	-71.056	109.337	1.00	27.71	B	N
	ATOM	3797	CA	TYR	328	-10.246	-69.831	109.111	1.00	29.17	B	C
40	ATOM	3798	CB	TYR	328	-10.460	-69.077	110.432	1.00	30.61	B	C
	ATOM	3799	CG	TYR	328	-11.094	-67.711	110.253	1.00	32.99	B	C
	ATOM	3800	CD1	TYR	328	-10.335	-66.618	109.826	1.00	33.59	B	C
	ATOM	3801	CE1	TYR	328	-10.921	-65.381	109.578	1.00	33.86	B	C
	ATOM	3802	CD2	TYR	328	-12.465	-67.524	110.437	1.00	34.14	B	C
45	ATOM	3803	CE2	TYR	328	-13.065	-66.281	110.191	1.00	34.54	B	C
	ATOM	3804	CZ	TYR	328	-12.284	-65.219	109.758	1.00	35.00	B	C
	ATOM	3805	OH	TYR	328	-12.864	-64.002	109.484	1.00	35.60	B	O
	ATOM	3806	C	TYR	328	-9.528	-68.936	108.099	1.00	29.11	B	C
	ATOM	3807	O	TYR	328	-10.163	-68.309	107.252	1.00	28.12	B	O
50	ATOM	3808	N	GLN	329	-8.204	-68.878	108.188	1.00	29.12	B	N
	ATOM	3809	CA	GLN	329	-7.416	-68.058	107.272	1.00	29.08	B	C
	ATOM	3810	CB	GLN	329	-5.936	-68.119	107.652	1.00	27.70	B	C
	ATOM	3811	CG	GLN	329	-5.613	-67.517	109.016	1.00	26.09	B	C
	ATOM	3812	CD	GLN	329	-5.914	-66.032	109.079	1.00	25.68	B	C
55	ATOM	3813	OE1	GLN	329	-6.717	-65.578	109.898	1.00	26.08	B	O
	ATOM	3814	NE2	GLN	329	-5.273	-65.267	108.209	1.00	24.01	B	N
	ATOM	3815	C	GLN	329	-7.584	-68.488	105.812	1.00	30.18	B	C
	ATOM	3816	O	GLN	329	-7.785	-67.649	104.932	1.00	29.17	B	O
	ATOM	3817	N	ILE	330	-7.508	-69.792	105.561	1.00	31.28	B	N
	ATOM	3818	CA	ILE	330	-7.632	-70.323	104.206	1.00	34.04	B	C
	ATOM	3819	CB	ILE	330	-7.138	-71.795	104.140	1.00	35.02	B	C
	ATOM	3820	CG2	ILE	330	-7.869	-72.640	105.155	1.00	36.98	B	C

-235-

5	ATOM	3821	CG1	ILE	330	-7.365	-72.370	102.738	1.00	36.93	B	C
	ATOM	3822	CD1	ILE	330	-6.811	-73.776	102.550	1.00	37.83	B	C
	ATOM	3823	C	ILE	330	-9.041	-70.233	103.600	1.00	34.84	B	C
	ATOM	3824	O	ILE	330	-9.194	-70.200	102.380	1.00	33.41	B	O
	ATOM	3825	N	GLN	331	-10.064	-70.199	104.447	1.00	36.52	B	N
10	ATOM	3826	CA	GLN	331	-11.435	-70.100	103.965	1.00	39.11	B	C
	ATOM	3827	CB	GLN	331	-12.414	-70.754	104.955	1.00	41.52	B	C
	ATOM	3828	CG	GLN	331	-12.738	-72.221	104.665	1.00	45.93	B	C
	ATOM	3829	CD	GLN	331	-11.691	-73.190	105.190	1.00	48.62	B	C
	ATOM	3830	OE1	GLN	331	-11.565	-73.397	106.400	1.00	50.00	B	O
15	ATOM	3831	NE2	GLN	331	-10.934	-73.793	104.278	1.00	50.06	B	N
	ATOM	3832	C	GLN	331	-11.856	-68.651	103.741	1.00	38.77	B	C
	ATOM	3833	O	GLN	331	-12.764	-68.380	102.962	1.00	39.36	B	O
	ATOM	3834	N	HIS	332	-11.188	-67.719	104.408	1.00	38.40	B	N
	ATOM	3835	CA	HIS	332	-11.552	-66.316	104.290	1.00	38.62	B	C
20	ATOM	3836	CB	HIS	332	-11.752	-65.742	105.690	1.00	40.74	B	C
	ATOM	3837	CG	HIS	332	-12.988	-66.250	106.368	1.00	43.93	B	C
	ATOM	3838	CD2	HIS	332	-13.214	-67.384	107.075	1.00	44.81	B	C
	ATOM	3839	ND1	HIS	332	-14.197	-65.591	106.304	1.00	44.67	B	N
	ATOM	3840	CE1	HIS	332	-15.115	-66.296	106.944	1.00	45.90	B	C
25	ATOM	3841	NE2	HIS	332	-14.544	-67.389	107.419	1.00	45.60	B	N
	ATOM	3842	C	HIS	332	-10.625	-65.418	103.477	1.00	37.56	B	C
	ATOM	3843	O	HIS	332	-10.985	-64.287	103.146	1.00	36.45	B	O
	ATOM	3844	N	ILE	333	-9.439	-65.915	103.146	1.00	36.43	B	N
	ATOM	3845	CA	ILE	333	-8.492	-65.130	102.369	1.00	35.55	B	C
30	ATOM	3846	CB	ILE	333	-7.243	-64.817	103.194	1.00	35.40	B	C
	ATOM	3847	CG2	ILE	333	-6.221	-64.090	102.338	1.00	35.90	B	C
	ATOM	3848	CG1	ILE	333	-7.644	-63.954	104.392	1.00	35.38	B	C
	ATOM	3849	CD1	ILE	333	-6.720	-64.060	105.558	1.00	35.02	B	C
	ATOM	3850	C	ILE	333	-8.111	-65.870	101.097	1.00	35.05	B	C
35	ATOM	3851	O	ILE	333	-7.275	-66.777	101.108	1.00	34.80	B	O
	ATOM	3852	N	GLN	334	-8.750	-65.470	100.003	1.00	33.98	B	N
	ATOM	3853	CA	GLN	334	-8.534	-66.072	98.698	1.00	33.55	B	C
	ATOM	3854	CB	GLN	334	-9.308	-65.284	97.635	1.00	34.76	B	C
	ATOM	3855	CG	GLN	334	-9.442	-65.984	96.293	1.00	37.74	B	C
40	ATOM	3856	CD	GLN	334	-10.199	-65.145	95.267	1.00	39.77	B	C
	ATOM	3857	OE1	GLN	334	-9.608	-64.335	94.550	1.00	40.63	B	O
	ATOM	3858	NE2	GLN	334	-11.516	-65.329	95.205	1.00	41.05	B	N
	ATOM	3859	C	GLN	334	-7.055	-66.101	98.347	1.00	31.83	B	C
	ATOM	3860	O	GLN	334	-6.355	-65.106	98.507	1.00	30.79	B	O
45	ATOM	3861	N	GLY	335	-6.581	-67.250	97.879	1.00	30.86	B	N
	ATOM	3862	CA	GLY	335	-5.183	-67.356	97.498	1.00	30.05	B	C
	ATOM	3863	C	GLY	335	-4.273	-68.065	98.481	1.00	29.05	B	C
	ATOM	3864	O	GLY	335	-3.315	-68.703	98.065	1.00	28.90	B	O
	ATOM	3865	N	LEU	336	-4.556	-67.964	99.777	1.00	28.28	B	N
50	ATOM	3866	CA	LEU	336	-3.720	-68.631	100.772	1.00	28.50	B	C
	ATOM	3867	CB	LEU	336	-4.228	-68.352	102.189	1.00	26.88	B	C
	ATOM	3868	CG	LEU	336	-3.993	-66.961	102.775	1.00	26.76	B	C
	ATOM	3869	CD1	LEU	336	-4.552	-66.906	104.198	1.00	25.90	B	C
	ATOM	3870	CD2	LEU	336	-2.506	-66.653	102.781	1.00	26.43	B	C
55	ATOM	3871	C	LEU	336	-3.635	-70.147	100.561	1.00	28.85	B	C
	ATOM	3872	O	LEU	336	-2.573	-70.744	100.761	1.00	28.06	B	O
	ATOM	3873	N	SER	337	-4.744	-70.761	100.149	1.00	29.32	B	N
	ATOM	3874	CA	SER	337	-4.795	-72.208	99.923	1.00	30.16	B	C
	ATOM	3875	CB	SER	337	-6.202	-72.631	99.482	1.00	30.24	B	C
	ATOM	3876	OG	SER	337	-6.551	-72.034	98.244	1.00	32.83	B	O
	ATOM	3877	C	SER	337	-3.771	-72.704	98.902	1.00	29.96	B	C
	ATOM	3878	O	SER	337	-3.374	-73.869	98.931	1.00	30.50	B	O

-236-

	ATOM	3879	N	ALA	338	-3.354	-71.828	97.996	1.00	29.75	B	N
	ATOM	3880	CA	ALA	338	-2.366	-72.188	96.983	1.00	30.35	B	C
	ATOM	3881	CB	ALA	338	-2.134	-71.015	96.043	1.00	29.79	B	C
5	ATOM	3882	C	ALA	338	-1.041	-72.615	97.615	1.00	30.54	B	C
	ATOM	3883	O	ALA	338	-0.306	-73.408	97.037	1.00	31.26	B	O
	ATOM	3884	N	MET	339	-0.736	-72.082	98.796	1.00	30.39	B	N
	ATOM	3885	CA	MET	339	0.499	-72.427	99.494	1.00	31.18	B	C
	ATOM	3886	CB	MET	339	0.906	-71.293	100.443	1.00	28.38	B	C
10	ATOM	3887	CG	MET	339	1.428	-70.061	99.719	1.00	27.58	B	C
	ATOM	3888	SD	MET	339	1.777	-68.662	100.804	1.00	25.78	B	S
	ATOM	3889	CE	MET	339	0.137	-67.932	100.914	1.00	26.72	B	C
	ATOM	3890	C	MET	339	0.399	-73.742	100.267	1.00	33.29	B	C
	ATOM	3891	O	MET	339	1.405	-74.253	100.758	1.00	32.44	B	O
15	ATOM	3892	N	MET	340	-0.810	-74.283	100.389	1.00	36.51	B	N
	ATOM	3893	CA	MET	340	-0.993	-75.546	101.091	1.00	41.83	B	C
	ATOM	3894	CB	MET	340	-2.462	-75.740	101.480	1.00	43.44	B	C
	ATOM	3895	CG	MET	340	-2.713	-76.879	102.469	1.00	46.96	B	C
	ATOM	3896	SD	MET	340	-1.738	-76.795	104.011	1.00	50.06	B	S
20	ATOM	3897	CE	MET	340	-1.302	-78.542	104.259	1.00	49.89	B	C
	ATOM	3898	C	MET	340	-0.533	-76.639	100.126	1.00	44.42	B	C
	ATOM	3899	O	MET	340	-1.034	-76.737	99.008	1.00	43.85	B	O
	ATOM	3900	N	PRO	341	0.441	-77.463	100.556	1.00	47.61	B	N
	ATOM	3901	CD	PRO	341	0.791	-77.444	101.990	1.00	48.17	B	C
25	ATOM	3902	CA	PRO	341	1.115	-78.593	99.902	1.00	50.66	B	C
	ATOM	3903	CB	PRO	341	1.434	-79.506	101.076	1.00	49.85	B	C
	ATOM	3904	CG	PRO	341	1.857	-78.525	102.094	1.00	48.96	B	C
	ATOM	3905	C	PRO	341	0.470	-79.352	98.734	1.00	53.61	B	C
	ATOM	3906	O	PRO	341	1.190	-79.959	97.932	1.00	53.85	B	O
30	ATOM	3907	N	LEU	342	-0.860	-79.329	98.640	1.00	56.59	B	N
	ATOM	3908	CA	LEU	342	-1.595	-80.017	97.575	1.00	59.91	B	C
	ATOM	3909	CB	LEU	342	-0.835	-79.921	96.241	1.00	59.68	B	C
	ATOM	3910	CG	LEU	342	-1.238	-80.824	95.070	1.00	59.94	B	C
	ATOM	3911	CD1	LEU	342	-0.926	-80.135	93.752	1.00	59.43	B	C
35	ATOM	3912	CD2	LEU	342	-0.506	-82.154	95.171	1.00	59.60	B	C
	ATOM	3913	C	LEU	342	-1.845	-81.475	97.949	1.00	62.30	B	C
	ATOM	3914	O	LEU	342	-2.944	-81.997	97.749	1.00	62.71	B	O
	ATOM	3915	N	LEU	343	-0.821	-82.126	98.493	1.00	64.97	B	N
	ATOM	3916	CA	LEU	343	-0.923	-83.516	98.922	1.00	67.52	B	C
40	ATOM	3917	CB	LEU	343	0.379	-83.961	99.600	1.00	67.63	B	C
	ATOM	3918	CG	LEU	343	1.710	-83.566	98.956	1.00	67.80	B	C
	ATOM	3919	CD1	LEU	343	2.846	-84.029	99.847	1.00	67.88	B	C
	ATOM	3920	CD2	LEU	343	1.828	-84.171	97.567	1.00	67.91	B	C
	ATOM	3921	C	LEU	343	-2.066	-83.599	99.932	1.00	68.96	B	C
45	ATOM	3922	O	LEU	343	-3.019	-84.362	99.758	1.00	68.99	B	O
	ATOM	3923	N	GLN	344	-1.950	-82.794	100.985	1.00	70.83	B	N
	ATOM	3924	CA	GLN	344	-2.944	-82.737	102.048	1.00	72.62	B	C
	ATOM	3925	CB	GLN	344	-2.496	-81.747	103.128	1.00	72.48	B	C
	ATOM	3926	CG	GLN	344	-1.098	-82.006	103.663	1.00	72.55	B	C
	ATOM	3927	CD	GLN	344	-1.003	-83.308	104.428	1.00	72.59	B	C
50	ATOM	3928	OE1	GLN	344	-1.517	-83.424	105.540	1.00	72.49	B	O
	ATOM	3929	NE2	GLN	344	-0.353	-84.301	103.832	1.00	72.52	B	N
	ATOM	3930	C	GLN	344	-4.299	-82.313	101.495	1.00	73.91	B	C
	ATOM	3931	O	GLN	344	-5.312	-82.970	101.740	1.00	74.16	B	O
55	ATOM	3932	N	GLU	345	-4.312	-81.214	100.745	1.00	75.31	B	N
	ATOM	3933	CA	GLU	345	-5.547	-80.701	100.166	1.00	76.49	B	C
	ATOM	3934	CB	GLU	345	-6.467	-80.214	101.288	1.00	77.05	B	C
	ATOM	3935	CG	GLU	345	-7.864	-79.823	100.846	1.00	77.78	B	C
	ATOM	3936	CD	GLU	345	-8.705	-79.330	102.005	1.00	78.25	B	C

-237-

5	ATOM	3937	OE1	GLU	345	-8.867	-80.087	102.987	1.00	78.37	B	O
	ATOM	3938	OE2	GLU	345	-9.200	-78.184	101.937	1.00	78.57	B	O
	ATOM	3939	C	GLU	345	-5.258	-79.557	99.193	1.00	76.87	B	C
	ATOM	3940	O	GLU	345	-5.484	-79.744	97.978	1.00	77.22	B	O
	ATOM	3941	OXT	GLU	345	-4.802	-78.490	99.657	1.00	77.25	B	O
10	TER	3942		GLU	345						B	
	ATOM	3943	CB	PRO	103	17.203	-24.177	122.780	1.00	92.75	C	C
	ATOM	3944	CG	PRO	103	15.916	-24.008	121.973	1.00	93.01	C	C
	ATOM	3945	C	PRO	103	16.591	-26.001	124.396	1.00	92.31	C	C
	ATOM	3946	O	PRO	103	15.433	-26.410	124.489	1.00	92.32	C	O
15	ATOM	3947	N	PRO	103	16.430	-26.298	121.930	1.00	92.88	C	N
	ATOM	3948	CD	PRO	103	15.865	-25.248	121.064	1.00	93.06	C	C
	ATOM	3949	CA	PRO	103	17.200	-25.678	123.033	1.00	92.61	C	C
	ATOM	3950	N	VAL	104	17.381	-25.812	125.450	1.00	91.79	C	N
	ATOM	3951	CA	VAL	104	16.934	-26.091	126.812	1.00	91.07	C	C
20	ATOM	3952	CB	VAL	104	17.809	-27.204	127.462	1.00	91.34	C	C
	ATOM	3953	CG1	VAL	104	17.551	-28.535	126.766	1.00	91.17	C	C
	ATOM	3954	CG2	VAL	104	19.289	-26.854	127.359	1.00	91.18	C	C
	ATOM	3955	C	VAL	104	16.946	-24.835	127.691	1.00	90.40	C	C
	ATOM	3956	O	VAL	104	17.957	-24.495	128.310	1.00	90.36	C	O
25	ATOM	3957	N	GLN	105	15.803	-24.156	127.742	1.00	89.40	C	N
	ATOM	3958	CA	GLN	105	15.652	-22.928	128.519	1.00	88.14	C	C
	ATOM	3959	CB	GLN	105	14.585	-22.028	127.879	1.00	88.78	C	C
	ATOM	3960	CG	GLN	105	15.024	-21.256	126.631	1.00	89.73	C	C
	ATOM	3961	CD	GLN	105	15.344	-22.145	125.438	1.00	90.20	C	C
30	ATOM	3962	OE1	GLN	105	16.377	-22.817	125.406	1.00	90.33	C	O
	ATOM	3963	NE2	GLN	105	14.454	-22.150	124.450	1.00	90.48	C	N
	ATOM	3964	C	GLN	105	15.274	-23.196	129.975	1.00	86.74	C	C
	ATOM	3965	O	GLN	105	15.063	-24.345	130.372	1.00	87.04	C	O
	ATOM	3966	N	LEU	106	15.193	-22.125	130.763	1.00	84.58	C	N
35	ATOM	3967	CA	LEU	106	14.831	-22.211	132.176	1.00	82.19	C	C
	ATOM	3968	CB	LEU	106	15.748	-23.199	132.907	1.00	82.41	C	C
	ATOM	3969	CG	LEU	106	15.400	-23.542	134.361	1.00	82.27	C	C
	ATOM	3970	CD1	LEU	106	13.961	-24.027	134.458	1.00	82.05	C	C
	ATOM	3971	CD2	LEU	106	16.356	-24.611	134.870	1.00	82.24	C	C
40	ATOM	3972	C	LEU	106	14.920	-20.833	132.834	1.00	80.39	C	C
	ATOM	3973	O	LEU	106	15.976	-20.432	133.322	1.00	80.25	C	O
	ATOM	3974	N	SER	107	13.798	-20.118	132.833	1.00	78.12	C	N
	ATOM	3975	CA	SER	107	13.698	-18.781	133.413	1.00	75.92	C	C
	ATOM	3976	CB	SER	107	12.229	-18.437	133.670	1.00	75.50	C	C
45	ATOM	3977	OG	SER	107	12.106	-17.218	134.377	1.00	74.70	C	O
	ATOM	3978	C	SER	107	14.484	-18.613	134.708	1.00	74.75	C	C
	ATOM	3979	O	SER	107	14.622	-19.552	135.491	1.00	74.59	C	O
	ATOM	3980	N	LYS	108	14.998	-17.405	134.927	1.00	73.23	C	N
	ATOM	3981	CA	LYS	108	15.761	-17.109	136.134	1.00	71.45	C	C
50	ATOM	3982	CB	LYS	108	16.580	-15.825	135.954	1.00	71.64	C	C
	ATOM	3983	CG	LYS	108	15.752	-14.553	135.829	1.00	71.83	C	C
	ATOM	3984	CD	LYS	108	16.621	-13.317	135.598	1.00	72.24	C	C
	ATOM	3985	CE	LYS	108	17.070	-13.171	134.142	1.00	72.27	C	C
	ATOM	3986	NZ	LYS	108	18.040	-14.211	133.689	1.00	72.65	C	N
55	ATOM	3987	C	LYS	108	14.828	-16.966	137.334	1.00	70.06	C	C
	ATOM	3988	O	LYS	108	15.241	-17.172	138.475	1.00	69.77	C	O
	ATOM	3989	N	GLU	109	13.572	-16.611	137.074	1.00	68.53	C	N
	ATOM	3990	CA	GLU	109	12.589	-16.460	138.139	1.00	66.79	C	C
	ATOM	3991	CB	GLU	109	11.342	-15.742	137.627	1.00	67.72	C	C
	ATOM	3992	CG	GLU	109	10.312	-15.496	138.709	1.00	69.22	C	C
	ATOM	3993	CD	GLU	109	9.117	-14.715	138.212	1.00	70.31	C	C
	ATOM	3994	OE1	GLU	109	9.308	-13.573	137.740	1.00	70.89	C	O

-238-

5	ATOM	3995	OE2	GLU	109	7.988	-15.245	138.297	1.00	71.04	C	O
	ATOM	3996	C	GLU	109	12.201	-17.832	138.678	1.00	64.99	C	C
	ATOM	3997	O	GLU	109	12.046	-18.013	139.887	1.00	64.83	C	O
	ATOM	3998	N	GLN	110	12.037	-18.799	137.782	1.00	62.56	C	N
	ATOM	3999	CA	GLN	110	11.694	-20.138	138.220	1.00	60.51	C	C
10	ATOM	4000	CB	GLN	110	11.100	-20.952	137.066	1.00	60.12	C	C
	ATOM	4001	CG	GLN	110	11.953	-21.069	135.821	1.00	59.34	C	C
	ATOM	4002	CD	GLN	110	11.148	-21.510	134.607	1.00	58.88	C	C
	ATOM	4003	OE1	GLN	110	11.714	-21.900	133.587	1.00	58.96	C	O
	ATOM	4004	NE2	GLN	110	9.822	-21.438	134.709	1.00	58.28	C	N
15	ATOM	4005	C	GLN	110	12.921	-20.818	138.830	1.00	59.45	C	C
	ATOM	4006	O	GLN	110	12.791	-21.798	139.561	1.00	59.18	C	O
	ATOM	4007	N	GLU	111	14.113	-20.297	138.538	1.00	57.98	C	N
	ATOM	4008	CA	GLU	111	15.330	-20.840	139.139	1.00	56.65	C	C
	ATOM	4009	CB	GLU	111	16.597	-20.256	138.501	1.00	57.99	C	C
20	ATOM	4010	CG	GLU	111	16.945	-20.813	137.131	1.00	59.95	C	C
	ATOM	4011	CD	GLU	111	18.446	-20.842	136.885	1.00	61.39	C	C
	ATOM	4012	OE1	GLU	111	19.107	-19.808	137.121	1.00	61.89	C	O
	ATOM	4013	OE2	GLU	111	18.966	-21.897	136.453	1.00	61.84	C	O
	ATOM	4014	C	GLU	111	15.289	-20.443	140.613	1.00	54.63	C	C
25	ATOM	4015	O	GLU	111	15.711	-21.203	141.478	1.00	54.15	C	O
	ATOM	4016	N	GLU	112	14.781	-19.241	140.881	1.00	52.67	C	N
	ATOM	4017	CA	GLU	112	14.641	-18.728	142.240	1.00	51.06	C	C
	ATOM	4018	CB	GLU	112	14.063	-17.306	142.209	1.00	52.04	C	C
	ATOM	4019	CG	GLU	112	13.553	-16.804	143.560	1.00	53.83	C	C
30	ATOM	4020	CD	GLU	112	14.667	-16.501	144.552	1.00	55.38	C	C
	ATOM	4021	OE1	GLU	112	15.678	-17.239	144.575	1.00	56.05	C	O
	ATOM	4022	OE2	GLU	112	14.523	-15.527	145.324	1.00	56.06	C	O
	ATOM	4023	C	GLU	112	13.703	-19.648	143.022	1.00	48.98	C	C
	ATOM	4024	O	GLU	112	13.994	-20.042	144.149	1.00	48.54	C	O
35	ATOM	4025	N	LEU	113	12.570	-19.973	142.409	1.00	46.59	C	N
	ATOM	4026	CA	LEU	113	11.582	-20.852	143.013	1.00	43.90	C	C
	ATOM	4027	CB	LEU	113	10.434	-21.086	142.030	1.00	43.46	C	C
	ATOM	4028	CG	LEU	113	9.345	-22.084	142.419	1.00	42.93	C	C
	ATOM	4029	CD1	LEU	113	8.648	-21.626	143.685	1.00	41.97	C	C
40	ATOM	4030	CD2	LEU	113	8.351	-22.210	141.272	1.00	42.66	C	C
	ATOM	4031	C	LEU	113	12.225	-22.181	143.396	1.00	42.33	C	C
	ATOM	4032	O	LEU	113	12.042	-22.672	144.502	1.00	41.47	C	O
	ATOM	4033	N	ILE	114	12.978	-22.768	142.476	1.00	41.11	C	N
	ATOM	4034	CA	ILE	114	13.640	-24.031	142.766	1.00	40.20	C	C
45	ATOM	4035	CB	ILE	114	14.374	-24.579	141.521	1.00	39.72	C	C
	ATOM	4036	CG2	ILE	114	15.231	-25.775	141.902	1.00	39.64	C	C
	ATOM	4037	CG1	ILE	114	13.350	-24.987	140.458	1.00	40.14	C	C
	ATOM	4038	CD1	ILE	114	13.957	-25.635	139.226	1.00	39.70	C	C
	ATOM	4039	C	ILE	114	14.636	-23.858	143.914	1.00	39.98	C	C
50	ATOM	4040	O	ILE	114	14.757	-24.724	144.782	1.00	39.82	C	O
	ATOM	4041	N	ARG	115	15.346	-22.735	143.916	1.00	39.67	C	N
	ATOM	4042	CA	ARG	115	16.323	-22.452	144.956	1.00	39.67	C	C
	ATOM	4043	CB	ARG	115	17.021	-21.116	144.670	1.00	41.84	C	C
	ATOM	4044	CG	ARG	115	18.199	-20.795	145.596	1.00	45.10	C	C
55	ATOM	4045	CD	ARG	115	17.743	-20.275	146.953	1.00	47.84	C	C
	ATOM	4046	NE	ARG	115	17.213	-18.914	146.880	1.00	50.53	C	N
	ATOM	4047	CZ	ARG	115	16.645	-18.272	147.901	1.00	52.18	C	C
	ATOM	4048	NH1	ARG	115	16.524	-18.862	149.086	1.00	52.65	C	N
	ATOM	4049	NH2	ARG	115	16.193	-17.035	147.739	1.00	52.40	C	N
	ATOM	4050	C	ARG	115	15.630	-22.410	146.315	1.00	37.89	C	C
	ATOM	4051	O	ARG	115	16.061	-23.069	147.260	1.00	37.73	C	O
	ATOM	4052	N	THR	116	14.552	-21.639	146.401	1.00	36.28	C	N

-239-

5	ATOM	4053	CA	THR	116	13.793	-21.512	147.633	1.00	34.60	C	C
	ATOM	4054	CB	THR	116	12.666	-20.439	147.475	1.00	35.71	C	C
	ATOM	4055	OG1	THR	116	11.901	-20.351	148.680	1.00	37.91	C	O
	ATOM	4056	CG2	THR	116	11.739	-20.776	146.334	1.00	37.42	C	C
	ATOM	4057	C	THR	116	13.220	-22.864	148.098	1.00	32.61	C	C
10	ATOM	4058	O	THR	116	13.281	-23.189	149.287	1.00	31.75	C	O
	ATOM	4059	N	LEU	117	12.692	-23.660	147.171	1.00	30.08	C	N
	ATOM	4060	CA	LEU	117	12.138	-24.971	147.518	1.00	28.36	C	C
	ATOM	4061	CB	LEU	117	11.458	-25.614	146.302	1.00	26.76	C	C
	ATOM	4062	CG	LEU	117	10.176	-24.967	145.769	1.00	25.75	C	C
15	ATOM	4063	CD1	LEU	117	9.678	-25.739	144.568	1.00	25.12	C	C
	ATOM	4064	CD2	LEU	117	9.114	-24.940	146.855	1.00	24.24	C	C
	ATOM	4065	C	LEU	117	13.233	-25.904	148.030	1.00	28.17	C	C
	ATOM	4066	O	LEU	117	13.052	-26.608	149.022	1.00	27.39	C	O
	ATOM	4067	N	LEU	118	14.370	-25.908	147.344	1.00	27.82	C	N
20	ATOM	4068	CA	LEU	118	15.498	-26.751	147.726	1.00	27.94	C	C
	ATOM	4069	CB	LEU	118	16.605	-26.639	146.673	1.00	28.74	C	C
	ATOM	4070	CG	LEU	118	16.745	-27.775	145.661	1.00	30.12	C	C
	ATOM	4071	CD1	LEU	118	15.403	-28.136	145.087	1.00	30.71	C	C
	ATOM	4072	CD2	LEU	118	17.711	-27.350	144.556	1.00	31.14	C	C
25	ATOM	4073	C	LEU	118	16.053	-26.383	149.105	1.00	27.07	C	C
	ATOM	4074	O	LEU	118	16.357	-27.255	149.913	1.00	26.71	C	O
	ATOM	4075	N	GLY	119	16.189	-25.090	149.366	1.00	26.49	C	N
	ATOM	4076	CA	GLY	119	16.699	-24.656	150.655	1.00	26.44	C	C
	ATOM	4077	C	GLY	119	15.815	-25.155	151.782	1.00	26.03	C	C
30	ATOM	4078	O	GLY	119	16.286	-25.806	152.714	1.00	25.94	C	O
	ATOM	4079	N	ALA	120	14.525	-24.850	151.694	1.00	25.49	C	N
	ATOM	4080	CA	ALA	120	13.560	-25.271	152.707	1.00	24.69	C	C
	ATOM	4081	CB	ALA	120	12.175	-24.774	152.329	1.00	24.54	C	C
	ATOM	4082	C	ALA	120	13.545	-26.793	152.858	1.00	24.27	C	C
35	ATOM	4083	O	ALA	120	13.555	-27.315	153.972	1.00	23.29	C	O
	ATOM	4084	N	HIS	121	13.521	-27.497	151.730	1.00	23.87	C	N
	ATOM	4085	CA	HIS	121	13.503	-28.953	151.733	1.00	23.41	C	C
	ATOM	4086	CB	HIS	121	13.385	-29.485	150.302	1.00	23.48	C	C
	ATOM	4087	CG	HIS	121	13.541	-30.969	150.197	1.00	23.06	C	C
40	ATOM	4088	CD2	HIS	121	12.654	-31.973	150.383	1.00	22.98	C	C
	ATOM	4089	ND1	HIS	121	14.742	-31.572	149.890	1.00	24.73	C	N
	ATOM	4090	CE1	HIS	121	14.587	-32.884	149.890	1.00	24.22	C	C
	ATOM	4091	NE2	HIS	121	13.329	-33.154	150.187	1.00	24.19	C	N
	ATOM	4092	C	HIS	121	14.743	-29.535	152.394	1.00	23.45	C	C
45	ATOM	4093	O	HIS	121	14.648	-30.426	153.230	1.00	22.84	C	O
	ATOM	4094	N	THR	122	15.912	-29.032	152.018	1.00	23.17	C	N
	ATOM	4095	CA	THR	122	17.152	-29.529	152.591	1.00	23.53	C	C
	ATOM	4096	CB	THR	122	18.379	-28.847	151.918	1.00	23.68	C	C
	ATOM	4097	OG1	THR	122	18.483	-29.298	150.560	1.00	23.80	C	O
50	ATOM	4098	CG2	THR	122	19.675	-29.195	152.657	1.00	23.99	C	C
	ATOM	4099	C	THR	122	17.193	-29.309	154.106	1.00	23.12	C	C
	ATOM	4100	O	THR	122	17.526	-30.215	154.872	1.00	22.20	C	O
	ATOM	4101	N	ARG	123	16.826	-28.110	154.535	1.00	22.95	C	N
	ATOM	4102	CA	ARG	123	16.843	-27.780	155.954	1.00	23.76	C	C
55	ATOM	4103	CB	ARG	123	16.591	-26.275	156.131	1.00	25.69	C	C
	ATOM	4104	CG	ARG	123	16.825	-25.737	157.549	1.00	28.57	C	C
	ATOM	4105	CD	ARG	123	16.329	-24.291	157.692	1.00	30.95	C	C
	ATOM	4106	NE	ARG	123	16.999	-23.365	156.775	1.00	33.62	C	N
	ATOM	4107	CZ	ARG	123	18.190	-22.807	156.996	1.00	34.51	C	C
	ATOM	4108	NH1	ARG	123	18.866	-23.066	158.111	1.00	33.79	C	N
	ATOM	4109	NH2	ARG	123	18.710	-21.982	156.095	1.00	34.90	C	N
	ATOM	4110	C	ARG	123	15.848	-28.560	156.819	1.00	22.89	C	C

-240-

5	ATOM	4111	O	ARG	123	16.173	-28.945	157.940	1.00	22.11	C	O
	ATOM	4112	N	HIS	124	14.651	-28.824	156.298	1.00	21.71	C	N
	ATOM	4113	CA	HIS	124	13.618	-29.483	157.101	1.00	21.10	C	C
	ATOM	4114	CB	HIS	124	12.399	-28.565	157.175	1.00	20.20	C	C
	ATOM	4115	CG	HIS	124	12.701	-27.207	157.718	1.00	19.38	C	C
10	ATOM	4116	CD2	HIS	124	13.214	-26.818	158.909	1.00	17.97	C	C
	ATOM	4117	ND1	HIS	124	12.473	-26.050	157.002	1.00	19.43	C	N
	ATOM	4118	CE1	HIS	124	12.832	-25.008	157.731	1.00	18.44	C	C
	ATOM	4119	NE2	HIS	124	13.285	-25.447	158.892	1.00	18.55	C	N
	ATOM	4120	C	HIS	124	13.108	-30.888	156.790	1.00	21.31	C	C
15	ATOM	4121	O	HIS	124	12.579	-31.555	157.684	1.00	20.78	C	O
	ATOM	4122	N	MET	125	13.253	-31.352	155.555	1.00	21.02	C	N
	ATOM	4123	CA	MET	125	12.715	-32.665	155.210	1.00	21.61	C	C
	ATOM	4124	CB	MET	125	11.498	-32.478	154.301	1.00	22.63	C	C
	ATOM	4125	CG	MET	125	10.436	-31.555	154.896	1.00	24.18	C	C
20	ATOM	4126	SD	MET	125	8.869	-31.737	154.075	1.00	26.74	C	S
	ATOM	4127	CE	MET	125	9.252	-31.067	152.446	1.00	26.67	C	C
	ATOM	4128	C	MET	125	13.659	-33.673	154.572	1.00	20.49	C	C
	ATOM	4129	O	MET	125	13.567	-34.860	154.856	1.00	19.83	C	O
	ATOM	4130	N	GLY	126	14.548	-33.195	153.706	1.00	20.13	C	N
25	ATOM	4131	CA	GLY	126	15.490	-34.063	153.015	1.00	19.93	C	C
	ATOM	4132	C	GLY	126	16.072	-35.193	153.840	1.00	20.19	C	C
	ATOM	4133	O	GLY	126	16.140	-36.333	153.376	1.00	19.39	C	O
	ATOM	4134	N	THR	127	16.495	-34.893	155.064	1.00	20.00	C	N
	ATOM	4135	CA	THR	127	17.070	-35.929	155.918	1.00	20.76	C	C
30	ATOM	4136	CB	THR	127	18.575	-35.664	156.155	1.00	20.73	C	C
	ATOM	4137	OG1	THR	127	18.755	-34.329	156.638	1.00	20.90	C	O
	ATOM	4138	CG2	THR	127	19.349	-35.824	154.850	1.00	19.98	C	C
	ATOM	4139	C	THR	127	16.369	-36.086	157.267	1.00	20.55	C	C
	ATOM	4140	O	THR	127	16.975	-36.534	158.245	1.00	19.57	C	O
35	ATOM	4141	N	MET	128	15.088	-35.739	157.318	1.00	20.36	C	N
	ATOM	4142	CA	MET	128	14.341	-35.846	158.566	1.00	20.82	C	C
	ATOM	4143	CB	MET	128	12.961	-35.193	158.419	1.00	21.34	C	C
	ATOM	4144	CG	MET	128	11.986	-35.955	157.523	1.00	21.05	C	C
	ATOM	4145	SD	MET	128	10.353	-35.170	157.462	1.00	20.70	C	S
40	ATOM	4146	CE	MET	128	9.538	-36.229	156.233	1.00	21.69	C	C
	ATOM	4147	C	MET	128	14.184	-37.297	159.019	1.00	20.76	C	C
	ATOM	4148	O	MET	128	14.025	-37.567	160.207	1.00	19.74	C	O
	ATOM	4149	N	PHE	129	14.239	-38.232	158.071	1.00	21.12	C	N
	ATOM	4150	CA	PHE	129	14.102	-39.648	158.386	1.00	21.43	C	C
45	ATOM	4151	CB	PHE	129	14.075	-40.472	157.089	1.00	23.16	C	C
	ATOM	4152	CG	PHE	129	15.407	-40.543	156.385	1.00	25.47	C	C
	ATOM	4153	CD1	PHE	129	16.397	-41.413	156.827	1.00	25.73	C	C
	ATOM	4154	CD2	PHE	129	15.677	-39.719	155.298	1.00	26.68	C	C
	ATOM	4155	CE1	PHE	129	17.637	-41.465	156.200	1.00	28.33	C	C
50	ATOM	4156	CE2	PHE	129	16.913	-39.758	154.661	1.00	27.60	C	C
	ATOM	4157	CZ	PHE	129	17.897	-40.632	155.112	1.00	28.66	C	C
	ATOM	4158	C	PHE	129	15.229	-40.150	159.300	1.00	20.85	C	C
	ATOM	4159	O	PHE	129	15.070	-41.163	159.983	1.00	19.76	C	O
	ATOM	4160	N	GLU	130	16.363	-39.450	159.314	1.00	20.93	C	N
55	ATOM	4161	CA	GLU	130	17.490	-39.860	160.153	1.00	22.74	C	C
	ATOM	4162	CB	GLU	130	18.728	-39.005	159.875	1.00	24.78	C	C
	ATOM	4163	CG	GLU	130	19.212	-39.056	158.446	1.00	27.92	C	C
	ATOM	4164	CD	GLU	130	20.438	-38.194	158.231	1.00	29.79	C	C
	ATOM	4165	OE1	GLU	130	20.672	-37.269	159.051	1.00	30.38	C	O
	ATOM	4166	OE2	GLU	130	21.157	-38.436	157.236	1.00	30.83	C	O
	ATOM	4167	C	GLU	130	17.176	-39.773	161.637	1.00	21.42	C	C
	ATOM	4168	O	GLU	130	17.855	-40.397	162.445	1.00	21.10	C	O

-241-

	ATOM	4169	N	GLN	131	16.152	-39.001	161.989	1.00	20.13	C	N
	ATOM	4170	CA	GLN	131	15.770	-38.843	163.382	1.00	20.44	C	C
	ATOM	4171	CB	GLN	131	15.199	-37.442	163.622	1.00	20.12	C	C
5	ATOM	4172	CG	GLN	131	16.162	-36.305	163.295	1.00	22.04	C	C
	ATOM	4173	CD	GLN	131	17.528	-36.478	163.949	1.00	22.44	C	C
	ATOM	4174	OE1	GLN	131	17.630	-36.726	165.156	1.00	20.89	C	O
	ATOM	4175	NE2	GLN	131	18.588	-36.347	163.149	1.00	21.74	C	N
	ATOM	4176	C	GLN	131	14.766	-39.880	163.878	1.00	20.14	C	C
10	ATOM	4177	O	GLN	131	14.500	-39.947	165.078	1.00	19.21	C	O
	ATOM	4178	N	PHE	132	14.211	-40.686	162.970	1.00	18.92	C	N
	ATOM	4179	CA	PHE	132	13.235	-41.709	163.360	1.00	18.44	C	C
	ATOM	4180	CB	PHE	132	12.850	-42.587	162.162	1.00	17.81	C	C
	ATOM	4181	CG	PHE	132	12.019	-41.883	161.104	1.00	18.33	C	C
15	ATOM	4182	CD1	PHE	132	11.560	-40.576	161.286	1.00	18.03	C	C
	ATOM	4183	CD2	PHE	132	11.692	-42.547	159.920	1.00	17.90	C	C
	ATOM	4184	CE1	PHE	132	10.788	-39.944	160.299	1.00	18.71	C	C
	ATOM	4185	CE2	PHE	132	10.927	-41.932	158.936	1.00	18.59	C	C
	ATOM	4186	CZ	PHE	132	10.472	-40.624	159.125	1.00	18.77	C	C
20	ATOM	4187	C	PHE	132	13.775	-42.607	164.478	1.00	18.64	C	C
	ATOM	4188	O	PHE	132	13.022	-43.061	165.353	1.00	16.29	C	O
	ATOM	4189	N	VAL	133	15.081	-42.866	164.446	1.00	18.83	C	N
	ATOM	4190	CA	VAL	133	15.699	-43.714	165.450	1.00	19.85	C	C
	ATOM	4191	CB	VAL	133	17.195	-43.995	165.102	1.00	20.35	C	C
25	ATOM	4192	CG1	VAL	133	18.012	-42.709	165.177	1.00	19.58	C	C
	ATOM	4193	CG2	VAL	133	17.758	-45.072	166.034	1.00	20.81	C	C
	ATOM	4194	C	VAL	133	15.589	-43.124	166.857	1.00	20.00	C	C
	ATOM	4195	O	VAL	133	15.698	-43.847	167.841	1.00	20.01	C	O
	ATOM	4196	N	GLN	134	15.345	-41.818	166.957	1.00	20.18	C	N
30	ATOM	4197	CA	GLN	134	15.228	-41.176	168.261	1.00	19.68	C	C
	ATOM	4198	CB	GLN	134	15.709	-39.717	168.187	1.00	20.98	C	C
	ATOM	4199	CG	GLN	134	17.111	-39.523	167.598	1.00	21.75	C	C
	ATOM	4200	CD	GLN	134	18.238	-40.182	168.411	1.00	24.09	C	C
	ATOM	4201	OE1	GLN	134	19.398	-40.190	167.982	1.00	25.24	C	O
35	ATOM	4202	NE2	GLN	134	17.906	-40.725	169.577	1.00	23.26	C	N
	ATOM	4203	C	GLN	134	13.819	-41.216	168.847	1.00	19.44	C	C
	ATOM	4204	O	GLN	134	13.577	-40.647	169.909	1.00	18.53	C	O
	ATOM	4205	N	PHE	135	12.897	-41.907	168.178	1.00	17.76	C	N
	ATOM	4206	CA	PHE	135	11.523	-41.994	168.656	1.00	17.30	C	C
40	ATOM	4207	CB	PHE	135	10.576	-41.420	167.599	1.00	16.60	C	C
	ATOM	4208	CG	PHE	135	10.665	-39.927	167.467	1.00	15.94	C	C
	ATOM	4209	CD1	PHE	135	10.059	-39.098	168.406	1.00	15.05	C	C
	ATOM	4210	CD2	PHE	135	11.399	-39.348	166.432	1.00	16.21	C	C
	ATOM	4211	CE1	PHE	135	10.180	-37.705	168.323	1.00	16.31	C	C
45	ATOM	4212	CE2	PHE	135	11.530	-37.956	166.337	1.00	15.93	C	C
	ATOM	4213	CZ	PHE	135	10.917	-37.132	167.288	1.00	15.48	C	C
	ATOM	4214	C	PHE	135	11.050	-43.383	169.072	1.00	17.74	C	C
	ATOM	4215	O	PHE	135	10.028	-43.872	168.587	1.00	16.28	C	O
	ATOM	4216	N	ARG	136	11.794	-44.003	169.982	1.00	18.46	C	N
50	ATOM	4217	CA	ARG	136	11.462	-45.326	170.522	1.00	20.06	C	C
	ATOM	4218	CB	ARG	136	10.302	-45.207	171.516	1.00	20.96	C	C
	ATOM	4219	CG	ARG	136	10.512	-44.156	172.580	1.00	24.90	C	C
	ATOM	4220	CD	ARG	136	9.309	-44.032	173.505	1.00	26.50	C	C
	ATOM	4221	NE	ARG	136	8.169	-43.333	172.903	1.00	27.43	C	N
55	ATOM	4222	CZ	ARG	136	7.111	-42.918	173.598	1.00	27.58	C	C
	ATOM	4223	NH1	ARG	136	7.052	-43.137	174.903	1.00	27.65	C	N
	ATOM	4224	NH2	ARG	136	6.124	-42.262	173.001	1.00	27.78	C	N
	ATOM	4225	C	ARG	136	11.095	-46.386	169.489	1.00	19.43	C	C
	ATOM	4226	O	ARG	136	10.042	-47.008	169.585	1.00	20.16	C	O

-242-

5	ATOM	4227	N	PRO	137	11.953	-46.614	168.494	1.00	18.91	C	N
	ATOM	4228	CD	PRO	137	13.266	-46.014	168.185	1.00	18.50	C	C
	ATOM	4229	CA	PRO	137	11.586	-47.637	167.512	1.00	18.39	C	C
	ATOM	4230	CB	PRO	137	12.607	-47.421	166.406	1.00	18.19	C	C
	ATOM	4231	CG	PRO	137	13.844	-46.991	167.190	1.00	18.43	C	C
10	ATOM	4232	C	PRO	137	11.677	-49.037	168.119	1.00	18.32	C	C
	ATOM	4233	O	PRO	137	12.612	-49.338	168.849	1.00	17.61	C	O
	ATOM	4234	N	PRO	138	10.690	-49.903	167.845	1.00	18.18	C	N
	ATOM	4235	CD	PRO	138	9.406	-49.665	167.165	1.00	18.09	C	C
	ATOM	4236	CA	PRO	138	10.753	-51.259	168.407	1.00	18.53	C	C
15	ATOM	4237	CB	PRO	138	9.459	-51.905	167.905	1.00	19.26	C	C
	ATOM	4238	CG	PRO	138	8.525	-50.729	167.784	1.00	20.92	C	C
	ATOM	4239	C	PRO	138	12.008	-51.942	167.851	1.00	18.85	C	C
	ATOM	4240	O	PRO	138	12.479	-51.588	166.767	1.00	17.83	C	O
	ATOM	4241	N	ALA	139	12.543	-52.914	168.585	1.00	18.83	C	N
20	ATOM	4242	CA	ALA	139	13.763	-53.608	168.170	1.00	19.23	C	C
	ATOM	4243	CB	ALA	139	14.176	-54.610	169.249	1.00	19.24	C	C
	ATOM	4244	C	ALA	139	13.712	-54.314	166.811	1.00	20.00	C	C
	ATOM	4245	O	ALA	139	14.716	-54.355	166.090	1.00	19.18	C	O
	ATOM	4246	N	HIS	140	12.560	-54.870	166.448	1.00	19.64	C	N
25	ATOM	4247	CA	HIS	140	12.471	-55.586	165.180	1.00	20.90	C	C
	ATOM	4248	CB	HIS	140	11.131	-56.340	165.073	1.00	19.67	C	C
	ATOM	4249	CG	HIS	140	9.967	-55.479	164.690	1.00	20.46	C	C
	ATOM	4250	CD2	HIS	140	9.320	-55.333	163.508	1.00	20.20	C	C
	ATOM	4251	ND1	HIS	140	9.340	-54.632	165.577	1.00	19.33	C	N
30	ATOM	4252	CE1	HIS	140	8.357	-54.000	164.959	1.00	20.25	C	C
	ATOM	4253	NE2	HIS	140	8.324	-54.406	163.704	1.00	20.65	C	N
	ATOM	4254	C	HIS	140	12.712	-54.727	163.927	1.00	21.31	C	C
	ATOM	4255	O	HIS	140	12.852	-55.259	162.827	1.00	21.71	C	O
	ATOM	4256	N	LEU	141	12.787	-53.410	164.092	1.00	21.64	C	N
35	ATOM	4257	CA	LEU	141	13.027	-52.505	162.964	1.00	22.55	C	C
	ATOM	4258	CB	LEU	141	12.357	-51.156	163.223	1.00	21.20	C	C
	ATOM	4259	CG	LEU	141	10.852	-51.128	163.475	1.00	21.22	C	C
	ATOM	4260	CD1	LEU	141	10.411	-49.687	163.714	1.00	19.35	C	C
	ATOM	4261	CD2	LEU	141	10.117	-51.742	162.274	1.00	20.05	C	C
40	ATOM	4262	C	LEU	141	14.511	-52.244	162.672	1.00	23.75	C	C
	ATOM	4263	O	LEU	141	14.845	-51.656	161.647	1.00	23.76	C	O
	ATOM	4264	N	PHE	142	15.401	-52.677	163.560	1.00	24.92	C	N
	ATOM	4265	CA	PHE	142	16.825	-52.413	163.377	1.00	27.83	C	C
	ATOM	4266	CB	PHE	142	17.537	-52.409	164.733	1.00	26.48	C	C
45	ATOM	4267	CG	PHE	142	17.322	-51.158	165.535	1.00	26.04	C	C
	ATOM	4268	CD1	PHE	142	16.332	-51.098	166.508	1.00	26.71	C	C
	ATOM	4269	CD2	PHE	142	18.130	-50.047	165.340	1.00	25.71	C	C
	ATOM	4270	CE1	PHE	142	16.156	-49.944	167.283	1.00	26.31	C	C
	ATOM	4271	CE2	PHE	142	17.958	-48.892	166.107	1.00	25.93	C	C
50	ATOM	4272	CZ	PHE	142	16.971	-48.844	167.080	1.00	24.84	C	C
	ATOM	4273	C	PHE	142	17.610	-53.318	162.428	1.00	29.94	C	C
	ATOM	4274	O	PHE	142	17.383	-54.523	162.376	1.00	29.88	C	O
	ATOM	4275	N	ILE	143	18.547	-52.700	161.704	1.00	32.51	C	N
	ATOM	4276	CA	ILE	143	19.461	-53.355	160.756	1.00	35.12	C	C
55	ATOM	4277	CB	ILE	143	20.474	-54.283	161.497	1.00	35.28	C	C
	ATOM	4278	CG2	ILE	143	21.545	-54.779	160.519	1.00	34.76	C	C
	ATOM	4279	CG1	ILE	143	21.154	-53.510	162.632	1.00	35.53	C	C
	ATOM	4280	CD1	ILE	143	21.750	-52.182	162.192	1.00	36.82	C	C
	ATOM	4281	C	ILE	143	18.769	-54.149	159.657	1.00	36.64	C	C
	ATOM	4282	O	ILE	143	18.813	-53.768	158.483	1.00	36.19	C	O
	ATOM	4283	N	HIS	144	18.178	-55.279	160.030	1.00	38.21	C	N
	ATOM	4284	CA	HIS	144	17.429	-56.087	159.082	1.00	39.85	C	C

-243-

5	ATOM	4285	CB	HIS	144	18.102	-57.439	158.821	1.00	42.16	C	C
	ATOM	4286	CG	HIS	144	17.372	-58.290	157.821	1.00	44.99	C	C
	ATOM	4287	CD2	HIS	144	16.240	-58.062	157.112	1.00	45.85	C	C
	ATOM	4288	ND1	HIS	144	17.800	-59.550	157.460	1.00	46.31	C	N
	ATOM	4289	CE1	HIS	144	16.964	-60.061	156.572	1.00	46.80	C	C
10	ATOM	4290	NE2	HIS	144	16.008	-59.178	156.344	1.00	46.60	C	N
	ATOM	4291	C	HIS	144	16.073	-56.302	159.728	1.00	39.44	C	C
	ATOM	4292	O	HIS	144	15.977	-56.886	160.809	1.00	38.57	C	O
	ATOM	4293	N	HIS	145	15.026	-55.812	159.075	1.00	39.00	C	N
	ATOM	4294	CA	HIS	145	13.693	-55.972	159.615	1.00	39.08	C	C
15	ATOM	4295	CB	HIS	145	12.639	-55.528	158.596	1.00	38.43	C	C
	ATOM	4296	CG	HIS	145	11.260	-55.408	159.171	1.00	38.37	C	C
	ATOM	4297	CD2	HIS	145	10.551	-54.322	159.566	1.00	37.79	C	C
	ATOM	4298	ND1	HIS	145	10.461	-56.501	159.433	1.00	37.09	C	N
	ATOM	4299	CE1	HIS	145	9.321	-56.095	159.963	1.00	37.12	C	C
20	ATOM	4300	NE2	HIS	145	9.350	-54.777	160.056	1.00	37.13	C	N
	ATOM	4301	C	HIS	145	13.486	-57.436	159.988	1.00	39.30	C	C
	ATOM	4302	O	HIS	145	13.828	-58.343	159.223	1.00	38.89	C	O
	ATOM	4303	N	GLN	146	12.949	-57.650	161.185	1.00	38.87	C	N
	ATOM	4304	CA	GLN	146	12.670	-58.984	161.690	1.00	38.47	C	C
25	ATOM	4305	CB	GLN	146	13.343	-59.213	163.036	1.00	39.68	C	C
	ATOM	4306	CG	GLN	146	14.769	-59.681	162.991	1.00	41.08	C	C
	ATOM	4307	CD	GLN	146	15.286	-59.921	164.389	1.00	43.84	C	C
	ATOM	4308	OE1	GLN	146	15.597	-58.976	165.116	1.00	45.31	C	O
	ATOM	4309	NE2	GLN	146	15.348	-61.188	164.791	1.00	44.12	C	N
30	ATOM	4310	C	GLN	146	11.178	-59.107	161.887	1.00	37.20	C	C
	ATOM	4311	O	GLN	146	10.515	-58.161	162.303	1.00	37.37	C	O
	ATOM	4312	N	PRO	147	10.624	-60.284	161.600	1.00	35.99	C	N
	ATOM	4313	CD	PRO	147	11.236	-61.547	161.151	1.00	35.90	C	C
	ATOM	4314	CA	PRO	147	9.184	-60.423	161.788	1.00	34.04	C	C
35	ATOM	4315	CB	PRO	147	8.910	-61.840	161.291	1.00	34.54	C	C
	ATOM	4316	CG	PRO	147	10.202	-62.558	161.570	1.00	35.92	C	C
	ATOM	4317	C	PRO	147	8.786	-60.213	163.249	1.00	32.25	C	C
	ATOM	4318	O	PRO	147	9.419	-60.741	164.166	1.00	31.73	C	O
	ATOM	4319	N	LEU	148	7.754	-59.406	163.463	1.00	29.88	C	N
40	ATOM	4320	CA	LEU	148	7.265	-59.167	164.811	1.00	26.83	C	C
	ATOM	4321	CB	LEU	148	6.273	-58.001	164.808	1.00	27.33	C	C
	ATOM	4322	CG	LEU	148	5.665	-57.566	166.142	1.00	28.42	C	C
	ATOM	4323	CD1	LEU	148	6.773	-57.134	167.091	1.00	28.52	C	C
	ATOM	4324	CD2	LEU	148	4.681	-56.420	165.911	1.00	28.07	C	C
45	ATOM	4325	C	LEU	148	6.562	-60.478	165.156	1.00	24.35	C	C
	ATOM	4326	O	LEU	148	5.809	-61.013	164.344	1.00	22.45	C	O
	ATOM	4327	N	PRO	149	6.829	-61.037	166.342	1.00	22.72	C	N
	ATOM	4328	CD	PRO	149	7.849	-60.668	167.337	1.00	21.82	C	C
	ATOM	4329	CA	PRO	149	6.171	-62.301	166.704	1.00	21.92	C	C
50	ATOM	4330	CB	PRO	149	6.704	-62.579	168.107	1.00	20.94	C	C
	ATOM	4331	CG	PRO	149	8.085	-61.986	168.051	1.00	22.25	C	C
	ATOM	4332	C	PRO	149	4.645	-62.222	166.667	1.00	21.18	C	C
	ATOM	4333	O	PRO	149	4.060	-61.164	166.859	1.00	21.31	C	O
	ATOM	4334	N	THR	150	4.014	-63.362	166.427	1.00	20.81	C	N
55	ATOM	4335	CA	THR	150	2.564	-63.470	166.352	1.00	20.80	C	C
	ATOM	4336	CB	THR	150	2.152	-64.950	166.233	1.00	19.51	C	C
	ATOM	4337	OG1	THR	150	2.553	-65.453	164.951	1.00	17.95	C	O
	ATOM	4338	CG2	THR	150	0.649	-65.107	166.404	1.00	19.20	C	C
	ATOM	4339	C	THR	150	1.804	-62.850	167.532	1.00	21.88	C	C
	ATOM	4340	O	THR	150	0.861	-62.085	167.336	1.00	21.66	C	O
	ATOM	4341	N	LEU	151	2.209	-63.181	168.751	1.00	21.61	C	N
	ATOM	4342	CA	LEU	151	1.527	-62.669	169.931	1.00	21.32	C	C

-244-

5	ATOM	4343	CB	LEU	151	1.369	-63.796	170.964	1.00	20.79	C	C
	ATOM	4344	CG	LEU	151	0.492	-64.995	170.548	1.00	20.54	C	C
	ATOM	4345	CD1	LEU	151	0.460	-66.025	171.675	1.00	20.72	C	C
	ATOM	4346	CD2	LEU	151	-0.926	-64.530	170.233	1.00	19.30	C	C
	ATOM	4347	C	LEU	151	2.207	-61.455	170.567	1.00	21.12	C	C
10	ATOM	4348	O	LEU	151	1.812	-61.012	171.641	1.00	21.25	C	O
	ATOM	4349	N	ALA	152	3.225	-60.916	169.908	1.00	19.97	C	N
	ATOM	4350	CA	ALA	152	3.918	-59.751	170.433	1.00	19.76	C	C
	ATOM	4351	CB	ALA	152	5.205	-59.516	169.649	1.00	18.98	C	C
	ATOM	4352	C	ALA	152	3.022	-58.506	170.365	1.00	19.64	C	C
15	ATOM	4353	O	ALA	152	2.337	-58.267	169.370	1.00	18.40	C	O
	ATOM	4354	N	PRO	153	3.003	-57.705	171.439	1.00	19.90	C	N
	ATOM	4355	CD	PRO	153	3.636	-57.923	172.754	1.00	20.17	C	C
	ATOM	4356	CA	PRO	153	2.177	-56.495	171.446	1.00	20.12	C	C
	ATOM	4357	CB	PRO	153	2.503	-55.865	172.801	1.00	20.62	C	C
20	ATOM	4358	CG	PRO	153	2.784	-57.067	173.669	1.00	20.46	C	C
	ATOM	4359	C	PRO	153	2.555	-55.573	170.286	1.00	20.10	C	C
	ATOM	4360	O	PRO	153	3.734	-55.405	169.989	1.00	19.34	C	O
	ATOM	4361	N	VAL	154	1.558	-54.986	169.626	1.00	21.19	C	N
	ATOM	4362	CA	VAL	154	1.834	-54.071	168.522	1.00	22.10	C	C
25	ATOM	4363	CB	VAL	154	0.763	-54.191	167.388	1.00	23.65	C	C
	ATOM	4364	CG1	VAL	154	-0.590	-53.693	167.869	1.00	24.74	C	C
	ATOM	4365	CG2	VAL	154	1.201	-53.395	166.172	1.00	24.89	C	C
	ATOM	4366	C	VAL	154	1.900	-52.623	169.026	1.00	21.26	C	C
	ATOM	4367	O	VAL	154	2.306	-51.726	168.296	1.00	21.70	C	O
30	ATOM	4368	N	LEU	155	1.516	-52.408	170.284	1.00	20.70	C	N
	ATOM	4369	CA	LEU	155	1.529	-51.075	170.902	1.00	19.78	C	C
	ATOM	4370	CB	LEU	155	1.174	-51.188	172.393	1.00	19.93	C	C
	ATOM	4371	CG	LEU	155	1.175	-49.911	173.250	1.00	21.72	C	C
	ATOM	4372	CD1	LEU	155	0.235	-48.872	172.660	1.00	20.06	C	C
35	ATOM	4373	CD2	LEU	155	0.755	-50.257	174.681	1.00	21.99	C	C
	ATOM	4374	C	LEU	155	2.852	-50.304	170.726	1.00	18.83	C	C
	ATOM	4375	O	LEU	155	2.839	-49.121	170.406	1.00	19.02	C	O
	ATOM	4376	N	PRO	156	4.011	-50.954	170.942	1.00	18.50	C	N
	ATOM	4377	CD	PRO	156	4.302	-52.259	171.571	1.00	17.61	C	C
40	ATOM	4378	CA	PRO	156	5.246	-50.179	170.754	1.00	17.22	C	C
	ATOM	4379	CB	PRO	156	6.334	-51.174	171.141	1.00	16.78	C	C
	ATOM	4380	CG	PRO	156	5.652	-52.011	172.205	1.00	17.22	C	C
	ATOM	4381	C	PRO	156	5.400	-49.660	169.314	1.00	17.71	C	C
	ATOM	4382	O	PRO	156	5.870	-48.539	169.093	1.00	16.22	C	O
45	ATOM	4383	N	LEU	157	5.002	-50.479	168.342	1.00	16.66	C	N
	ATOM	4384	CA	LEU	157	5.084	-50.089	166.942	1.00	17.15	C	C
	ATOM	4385	CB	LEU	157	4.726	-51.267	166.019	1.00	15.68	C	C
	ATOM	4386	CG	LEU	157	4.779	-50.951	164.516	1.00	14.50	C	C
	ATOM	4387	CD1	LEU	157	6.147	-50.381	164.153	1.00	12.24	C	C
50	ATOM	4388	CD2	LEU	157	4.491	-52.203	163.714	1.00	11.45	C	C
	ATOM	4389	C	LEU	157	4.126	-48.932	166.688	1.00	16.47	C	C
	ATOM	4390	O	LEU	157	4.483	-47.971	166.016	1.00	16.30	C	O
	ATOM	4391	N	VAL	158	2.914	-49.039	167.229	1.00	16.36	C	N
	ATOM	4392	CA	VAL	158	1.895	-48.003	167.088	1.00	16.91	C	C
55	ATOM	4393	CB	VAL	158	0.565	-48.438	167.762	1.00	17.14	C	C
	ATOM	4394	CG1	VAL	158	-0.434	-47.291	167.732	1.00	15.19	C	C
	ATOM	4395	CG2	VAL	158	-0.014	-49.662	167.046	1.00	15.59	C	C
	ATOM	4396	C	VAL	158	2.370	-46.690	167.727	1.00	17.43	C	C
	ATOM	4397	O	VAL	158	2.211	-45.613	167.154	1.00	17.53	C	O
	ATOM	4398	N	THR	159	2.946	-46.782	168.919	1.00	16.70	C	N
	ATOM	4399	CA	THR	159	3.449	-45.595	169.605	1.00	17.05	C	C
	ATOM	4400	CB	THR	159	4.045	-45.956	170.976	1.00	16.94	C	C

-245-

5	ATOM	4401	OG1	THR	159	3.040	-46.585	171.776	1.00	15.26	C	O
	ATOM	4402	CG2	THR	159	4.547	-44.700	171.686	1.00	17.16	C	C
	ATOM	4403	C	THR	159	4.527	-44.930	168.755	1.00	16.11	C	C
	ATOM	4404	O	THR	159	4.539	-43.710	168.602	1.00	17.45	C	O
	ATOM	4405	N	HIS	160	5.426	-45.742	168.206	1.00	15.29	C	N
10	ATOM	4406	CA	HIS	160	6.509	-45.257	167.351	1.00	14.74	C	C
	ATOM	4407	CB	HIS	160	7.397	-46.430	166.912	1.00	14.28	C	C
	ATOM	4408	CG	HIS	160	8.445	-46.055	165.905	1.00	13.23	C	C
	ATOM	4409	CD2	HIS	160	8.627	-46.444	164.620	1.00	13.10	C	C
	ATOM	4410	ND1	HIS	160	9.462	-45.168	166.182	1.00	13.39	C	N
15	ATOM	4411	CE1	HIS	160	10.228	-45.027	165.112	1.00	13.13	C	C
	ATOM	4412	NE2	HIS	160	9.744	-45.792	164.151	1.00	12.34	C	N
	ATOM	4413	C	HIS	160	5.961	-44.541	166.116	1.00	14.39	C	C
	ATOM	4414	O	HIS	160	6.435	-43.463	165.757	1.00	14.03	C	O
	ATOM	4415	N	PHE	161	4.973	-45.144	165.458	1.00	14.40	C	N
20	ATOM	4416	CA	PHE	161	4.370	-44.526	164.280	1.00	15.29	C	C
	ATOM	4417	CB	PHE	161	3.348	-45.472	163.633	1.00	15.35	C	C
	ATOM	4418	CG	PHE	161	3.966	-46.510	162.706	1.00	17.07	C	C
	ATOM	4419	CD1	PHE	161	5.299	-46.417	162.313	1.00	15.87	C	C
	ATOM	4420	CD2	PHE	161	3.193	-47.558	162.199	1.00	17.11	C	C
25	ATOM	4421	CE1	PHE	161	5.857	-47.341	161.432	1.00	17.22	C	C
	ATOM	4422	CE2	PHE	161	3.742	-48.496	161.308	1.00	18.15	C	C
	ATOM	4423	CZ	PHE	161	5.077	-48.388	160.923	1.00	17.06	C	C
	ATOM	4424	C	PHE	161	3.703	-43.186	164.636	1.00	14.79	C	C
	ATOM	4425	O	PHE	161	3.864	-42.198	163.928	1.00	13.30	C	O
30	ATOM	4426	N	ALA	162	2.954	-43.156	165.732	1.00	15.09	C	N
	ATOM	4427	CA	ALA	162	2.314	-41.918	166.153	1.00	15.95	C	C
	ATOM	4428	CB	ALA	162	1.532	-42.135	167.440	1.00	15.00	C	C
	ATOM	4429	C	ALA	162	3.376	-40.835	166.358	1.00	15.56	C	C
	ATOM	4430	O	ALA	162	3.162	-39.687	165.986	1.00	15.40	C	O
35	ATOM	4431	N	ASP	163	4.521	-41.201	166.938	1.00	16.37	C	N
	ATOM	4432	CA	ASP	163	5.599	-40.232	167.165	1.00	17.11	C	C
	ATOM	4433	CB	ASP	163	6.709	-40.831	168.039	1.00	18.76	C	C
	ATOM	4434	CG	ASP	163	6.353	-40.851	169.518	1.00	19.80	C	C
	ATOM	4435	OD1	ASP	163	7.160	-41.385	170.303	1.00	20.29	C	O
40	ATOM	4436	OD2	ASP	163	5.277	-40.335	169.896	1.00	20.75	C	O
	ATOM	4437	C	ASP	163	6.228	-39.695	165.879	1.00	16.41	C	C
	ATOM	4438	O	ASP	163	6.317	-38.486	165.703	1.00	16.53	C	O
	ATOM	4439	N	ILE	164	6.663	-40.575	164.976	1.00	15.27	C	N
	ATOM	4440	CA	ILE	164	7.285	-40.093	163.747	1.00	14.57	C	C
45	ATOM	4441	CB	ILE	164	8.092	-41.214	163.018	1.00	14.61	C	C
	ATOM	4442	CG2	ILE	164	9.149	-41.783	163.974	1.00	12.74	C	C
	ATOM	4443	CG1	ILE	164	7.162	-42.312	162.497	1.00	13.93	C	C
	ATOM	4444	CD1	ILE	164	7.882	-43.380	161.668	1.00	15.42	C	C
	ATOM	4445	C	ILE	164	6.262	-39.452	162.801	1.00	14.37	C	C
50	ATOM	4446	O	ILE	164	6.601	-38.552	162.025	1.00	13.76	C	O
	ATOM	4447	N	ASN	165	5.012	-39.903	162.854	1.00	13.47	C	N
	ATOM	4448	CA	ASN	165	3.982	-39.281	162.018	1.00	14.22	C	C
	ATOM	4449	CB	ASN	165	2.622	-39.977	162.189	1.00	13.22	C	C
	ATOM	4450	CG	ASN	165	2.520	-41.304	161.424	1.00	13.80	C	C
55	ATOM	4451	OD1	ASN	165	3.333	-41.604	160.545	1.00	13.34	C	O
	ATOM	4452	ND2	ASN	165	1.496	-42.089	161.748	1.00	11.89	C	N
	ATOM	4453	C	ASN	165	3.847	-37.809	162.453	1.00	13.40	C	C
	ATOM	4454	O	ASN	165	3.753	-36.913	161.620	1.00	12.46	C	O
	ATOM	4455	N	THR	166	3.846	-37.572	163.764	1.00	14.10	C	N
	ATOM	4456	CA	THR	166	3.702	-36.220	164.302	1.00	15.32	C	C
	ATOM	4457	CB	THR	166	3.359	-36.270	165.807	1.00	16.12	C	C
	ATOM	4458	OG1	THR	166	2.204	-37.099	165.995	1.00	15.30	C	O

-246-

5	ATOM	4459	CG2	THR	166	3.055	-34.869	166.348	1.00	14.52	C	C
	ATOM	4460	C	THR	166	4.968	-35.403	164.064	1.00	15.86	C	C
	ATOM	4461	O	THR	166	4.903	-34.223	163.724	1.00	16.48	C	O
	ATOM	4462	N	PHE	167	6.124	-36.035	164.234	1.00	17.03	C	N
	ATOM	4463	CA	PHE	167	7.400	-35.373	163.990	1.00	16.78	C	C
10	ATOM	4464	CB	PHE	167	8.542	-36.363	164.247	1.00	17.79	C	C
	ATOM	4465	CG	PHE	167	9.869	-35.942	163.675	1.00	18.70	C	C
	ATOM	4466	CD1	PHE	167	10.606	-34.915	164.256	1.00	19.29	C	C
	ATOM	4467	CD2	PHE	167	10.392	-36.594	162.558	1.00	19.25	C	C
	ATOM	4468	CE1	PHE	167	11.851	-34.545	163.734	1.00	19.64	C	C
15	ATOM	4469	CE2	PHE	167	11.632	-36.234	162.030	1.00	19.87	C	C
	ATOM	4470	CZ	PHE	167	12.365	-35.208	162.617	1.00	19.58	C	C
	ATOM	4471	C	PHE	167	7.429	-34.887	162.532	1.00	16.84	C	C
	ATOM	4472	O	PHE	167	7.805	-33.744	162.251	1.00	16.80	C	O
	ATOM	4473	N	MET	168	7.033	-35.755	161.603	1.00	15.69	C	N
20	ATOM	4474	CA	MET	168	7.023	-35.397	160.187	1.00	14.91	C	C
	ATOM	4475	CB	MET	168	6.661	-36.608	159.312	1.00	14.73	C	C
	ATOM	4476	CG	MET	168	7.782	-37.634	159.161	1.00	12.77	C	C
	ATOM	4477	SD	MET	168	7.419	-38.898	157.918	1.00	13.46	C	S
	ATOM	4478	CE	MET	168	6.583	-40.139	158.891	1.00	9.89	C	C
25	ATOM	4479	C	MET	168	6.066	-34.251	159.890	1.00	15.70	C	C
	ATOM	4480	O	MET	168	6.382	-33.364	159.097	1.00	13.88	C	O
	ATOM	4481	N	VAL	169	4.889	-34.273	160.510	1.00	16.72	C	N
	ATOM	4482	CA	VAL	169	3.926	-33.202	160.303	1.00	17.84	C	C
	ATOM	4483	CB	VAL	169	2.638	-33.425	161.132	1.00	18.74	C	C
30	ATOM	4484	CG1	VAL	169	1.781	-32.169	161.111	1.00	16.96	C	C
	ATOM	4485	CG2	VAL	169	1.837	-34.588	160.544	1.00	17.94	C	C
	ATOM	4486	C	VAL	169	4.561	-31.863	160.694	1.00	18.62	C	C
	ATOM	4487	O	VAL	169	4.467	-30.885	159.954	1.00	18.14	C	O
	ATOM	4488	N	LEU	170	5.219	-31.819	161.850	1.00	19.05	C	N
35	ATOM	4489	CA	LEU	170	5.860	-30.584	162.284	1.00	18.80	C	C
	ATOM	4490	CB	LEU	170	6.419	-30.741	163.700	1.00	19.18	C	C
	ATOM	4491	CG	LEU	170	5.375	-30.939	164.808	1.00	20.13	C	C
	ATOM	4492	CD1	LEU	170	6.065	-31.306	166.112	1.00	20.19	C	C
	ATOM	4493	CD2	LEU	170	4.560	-29.665	164.983	1.00	21.80	C	C
40	ATOM	4494	C	LEU	170	6.964	-30.177	161.297	1.00	19.15	C	C
	ATOM	4495	O	LEU	170	7.167	-28.989	161.055	1.00	19.95	C	O
	ATOM	4496	N	GLN	171	7.670	-31.148	160.718	1.00	18.11	C	N
	ATOM	4497	CA	GLN	171	8.713	-30.819	159.743	1.00	17.90	C	C
	ATOM	4498	CB	GLN	171	9.557	-32.050	159.382	1.00	17.69	C	C
45	ATOM	4499	CG	GLN	171	10.492	-32.522	160.501	1.00	19.25	C	C
	ATOM	4500	CD	GLN	171	11.383	-31.408	161.040	1.00	19.45	C	C
	ATOM	4501	OE1	GLN	171	12.164	-30.802	160.305	1.00	21.44	C	O
	ATOM	4502	NE2	GLN	171	11.268	-31.138	162.328	1.00	19.42	C	N
	ATOM	4503	C	GLN	171	8.141	-30.207	158.458	1.00	17.82	C	C
50	ATOM	4504	O	GLN	171	8.793	-29.361	157.841	1.00	17.25	C	O
	ATOM	4505	N	VAL	172	6.951	-30.646	158.039	1.00	17.26	C	N
	ATOM	4506	CA	VAL	172	6.322	-30.097	156.834	1.00	18.43	C	C
	ATOM	4507	CB	VAL	172	5.085	-30.927	156.376	1.00	18.66	C	C
	ATOM	4508	CG1	VAL	172	4.422	-30.247	155.185	1.00	17.80	C	C
55	ATOM	4509	CG2	VAL	172	5.509	-32.333	155.967	1.00	18.65	C	C
	ATOM	4510	C	VAL	172	5.871	-28.654	157.107	1.00	18.42	C	C
	ATOM	4511	O	VAL	172	6.026	-27.773	156.264	1.00	18.24	C	O
	ATOM	4512	N	ILE	173	5.304	-28.416	158.286	1.00	18.42	C	N
	ATOM	4513	CA	ILE	173	4.874	-27.073	158.644	1.00	18.94	C	C
55	ATOM	4514	CB	ILE	173	4.315	-27.034	160.090	1.00	19.45	C	C
	ATOM	4515	CG2	ILE	173	4.136	-25.590	160.550	1.00	18.53	C	C
	ATOM	4516	CG1	ILE	173	2.976	-27.786	160.147	1.00	19.67	C	C

-247-

	ATOM	4517	CD1	ILE	173	2.460	-28.048	161.559	1.00	18.69	C	C
	ATOM	4518	C	ILE	173	6.077	-26.128	158.509	1.00	18.47	C	C
	ATOM	4519	O	ILE	173	5.984	-25.093	157.856	1.00	17.88	C	O
5	ATOM	4520	N	LYS	174	7.209	-26.498	159.103	1.00	17.67	C	N
	ATOM	4521	CA	LYS	174	8.410	-25.671	159.025	1.00	18.85	C	C
	ATOM	4522	CB	LYS	174	9.559	-26.325	159.797	1.00	19.84	C	C
	ATOM	4523	CG	LYS	174	9.282	-26.514	161.293	1.00	20.37	C	C
	ATOM	4524	CD	LYS	174	10.454	-27.203	161.996	1.00	22.31	C	C
10	ATOM	4525	CE	LYS	174	11.661	-26.287	162.080	1.00	24.43	C	C
	ATOM	4526	NZ	LYS	174	12.790	-26.910	162.841	1.00	27.02	C	N
	ATOM	4527	C	LYS	174	8.826	-25.447	157.568	1.00	19.16	C	C
	ATOM	4528	O	LYS	174	9.241	-24.349	157.194	1.00	18.69	C	O
	ATOM	4529	N	PHE	175	8.722	-26.499	156.758	1.00	18.61	C	N
15	ATOM	4530	CA	PHE	175	9.061	-26.432	155.342	1.00	18.87	C	C
	ATOM	4531	CB	PHE	175	8.850	-27.803	154.697	1.00	18.31	C	C
	ATOM	4532	CG	PHE	175	8.852	-27.776	153.190	1.00	18.11	C	C
	ATOM	4533	CD1	PHE	175	10.004	-27.434	152.485	1.00	16.75	C	C
	ATOM	4534	CD2	PHE	175	7.702	-28.099	152.478	1.00	17.31	C	C
20	ATOM	4535	CE1	PHE	175	10.009	-27.416	151.090	1.00	17.12	C	C
	ATOM	4536	CE2	PHE	175	7.697	-28.084	151.079	1.00	16.84	C	C
	ATOM	4537	CZ	PHE	175	8.854	-27.742	150.386	1.00	16.17	C	C
	ATOM	4538	C	PHE	175	8.201	-25.397	154.619	1.00	19.59	C	C
	ATOM	4539	O	PHE	175	8.718	-24.558	153.875	1.00	19.63	C	O
25	ATOM	4540	N	THR	176	6.889	-25.460	154.834	1.00	19.92	C	N
	ATOM	4541	CA	THR	176	5.977	-24.528	154.181	1.00	21.48	C	C
	ATOM	4542	CB	THR	176	4.491	-24.902	154.427	1.00	21.69	C	C
	ATOM	4543	OG1	THR	176	4.209	-24.860	155.833	1.00	22.61	C	O
	ATOM	4544	CG2	THR	176	4.184	-26.288	153.886	1.00	20.21	C	C
30	ATOM	4545	C	THR	176	6.197	-23.096	154.668	1.00	22.48	C	C
	ATOM	4546	O	THR	176	6.077	-22.146	153.896	1.00	22.19	C	O
	ATOM	4547	N	LYS	177	6.521	-22.938	155.946	1.00	22.93	C	N
	ATOM	4548	CA	LYS	177	6.742	-21.606	156.491	1.00	24.72	C	C
	ATOM	4549	CB	LYS	177	6.833	-21.662	158.018	1.00	25.60	C	C
35	ATOM	4550	CG	LYS	177	5.447	-21.769	158.658	1.00	28.46	C	C
	ATOM	4551	CD	LYS	177	5.470	-21.611	160.169	1.00	28.76	C	C
	ATOM	4552	CE	LYS	177	4.110	-21.959	160.754	1.00	28.66	C	C
	ATOM	4553	NZ	LYS	177	3.026	-21.100	160.208	1.00	29.61	C	N
	ATOM	4554	C	LYS	177	7.951	-20.884	155.900	1.00	24.56	C	C
40	ATOM	4555	O	LYS	177	8.032	-19.661	155.971	1.00	23.75	C	O
	ATOM	4556	N	ASP	178	8.879	-21.635	155.313	1.00	24.31	C	N
	ATOM	4557	CA	ASP	178	10.056	-21.039	154.684	1.00	25.00	C	C
	ATOM	4558	CB	ASP	178	11.275	-21.950	154.849	1.00	24.90	C	C
	ATOM	4559	CG	ASP	178	11.887	-21.859	156.238	1.00	25.48	C	C
45	ATOM	4560	OD1	ASP	178	11.313	-21.146	157.090	1.00	26.26	C	O
	ATOM	4561	OD2	ASP	178	12.933	-22.496	156.478	1.00	24.33	C	O
	ATOM	4562	C	ASP	178	9.822	-20.767	153.199	1.00	25.18	C	C
	ATOM	4563	O	ASP	178	10.764	-20.534	152.448	1.00	26.75	C	O
	ATOM	4564	N	LEU	179	8.564	-20.801	152.772	1.00	24.75	C	N
50	ATOM	4565	CA	LEU	179	8.234	-20.553	151.379	1.00	24.20	C	C
	ATOM	4566	CB	LEU	179	7.389	-21.700	150.822	1.00	23.10	C	C
	ATOM	4567	CG	LEU	179	8.029	-23.086	150.875	1.00	22.16	C	C
	ATOM	4568	CD1	LEU	179	7.108	-24.089	150.183	1.00	21.20	C	C
	ATOM	4569	CD2	LEU	179	9.401	-23.045	150.213	1.00	20.84	C	C
55	ATOM	4570	C	LEU	179	7.462	-19.250	151.264	1.00	24.41	C	C
	ATOM	4571	O	LEU	179	6.290	-19.187	151.623	1.00	24.15	C	O
	ATOM	4572	N	PRO	180	8.117	-18.185	150.776	1.00	25.02	C	N
	ATOM	4573	CD	PRO	180	9.546	-18.088	150.417	1.00	25.26	C	C
	ATOM	4574	CA	PRO	180	7.456	-16.886	150.627	1.00	25.07	C	C

-248-

5	ATOM	4575	CB	PRO	180	8.446	-16.102	149.771	1.00	25.45	C	C
	ATOM	4576	CG	PRO	180	9.757	-16.576	150.309	1.00	25.01	C	C
	ATOM	4577	C	PRO	180	6.062	-16.973	150.003	1.00	25.06	C	C
	ATOM	4578	O	PRO	180	5.107	-16.419	150.543	1.00	24.75	C	O
	ATOM	4579	N	VAL	181	5.937	-17.676	148.880	1.00	25.37	C	N
10	ATOM	4580	CA	VAL	181	4.637	-17.808	148.218	1.00	26.24	C	C
	ATOM	4581	CB	VAL	181	4.743	-18.624	146.898	1.00	27.68	C	C
	ATOM	4582	CG1	VAL	181	5.515	-17.822	145.857	1.00	28.55	C	C
	ATOM	4583	CG2	VAL	181	5.424	-19.971	147.151	1.00	28.30	C	C
	ATOM	4584	C	VAL	181	3.566	-18.439	149.113	1.00	25.72	C	C
15	ATOM	4585	O	VAL	181	2.384	-18.116	148.996	1.00	25.14	C	O
	ATOM	4586	N	PHE	182	3.981	-19.341	149.997	1.00	25.42	C	N
	ATOM	4587	CA	PHE	182	3.062	-19.988	150.933	1.00	25.66	C	C
	ATOM	4588	CB	PHE	182	3.737	-21.199	151.602	1.00	24.81	C	C
	ATOM	4589	CG	PHE	182	2.859	-21.923	152.598	1.00	24.52	C	C
20	ATOM	4590	CD1	PHE	182	1.909	-22.845	152.172	1.00	24.87	C	C
	ATOM	4591	CD2	PHE	182	2.991	-21.687	153.966	1.00	25.69	C	C
	ATOM	4592	CE1	PHE	182	1.103	-23.524	153.089	1.00	23.82	C	C
	ATOM	4593	CE2	PHE	182	2.185	-22.362	154.897	1.00	25.07	C	C
	ATOM	4594	CZ	PHE	182	1.240	-23.282	154.452	1.00	24.45	C	C
25	ATOM	4595	C	PHE	182	2.676	-18.971	152.006	1.00	25.40	C	C
	ATOM	4596	O	PHE	182	1.497	-18.796	152.311	1.00	24.95	C	O
	ATOM	4597	N	ARG	183	3.679	-18.303	152.575	1.00	25.82	C	N
	ATOM	4598	CA	ARG	183	3.450	-17.309	153.624	1.00	27.71	C	C
	ATOM	4599	CB	ARG	183	4.787	-16.809	154.191	1.00	26.21	C	C
30	ATOM	4600	CG	ARG	183	5.521	-17.831	155.048	1.00	25.37	C	C
	ATOM	4601	CD	ARG	183	4.739	-18.176	156.325	1.00	24.60	C	C
	ATOM	4602	NE	ARG	183	4.826	-17.143	157.362	1.00	24.49	C	N
	ATOM	4603	CZ	ARG	183	5.922	-16.855	158.063	1.00	23.34	C	C
	ATOM	4604	NH1	ARG	183	7.052	-17.518	157.858	1.00	22.74	C	N
35	ATOM	4605	NH2	ARG	183	5.885	-15.900	158.981	1.00	23.81	C	N
	ATOM	4606	C	ARG	183	2.605	-16.107	153.201	1.00	28.86	C	C
	ATOM	4607	O	ARG	183	2.001	-15.455	154.049	1.00	29.70	C	O
	ATOM	4608	N	SER	184	2.558	-15.811	151.904	1.00	30.04	C	N
	ATOM	4609	CA	SER	184	1.775	-14.678	151.418	1.00	31.75	C	C
40	ATOM	4610	CB	SER	184	2.271	-14.236	150.038	1.00	32.20	C	C
	ATOM	4611	OG	SER	184	2.237	-15.312	149.121	1.00	35.11	C	O
	ATOM	4612	C	SER	184	0.280	-14.972	151.352	1.00	32.31	C	C
	ATOM	4613	O	SER	184	-0.536	-14.052	151.266	1.00	33.12	C	O
	ATOM	4614	N	LEU	185	-0.086	-16.249	151.388	1.00	32.24	C	N
45	ATOM	4615	CA	LEU	185	-1.492	-16.625	151.344	1.00	32.23	C	C
	ATOM	4616	CB	LEU	185	-1.636	-18.113	151.018	1.00	31.74	C	C
	ATOM	4617	CG	LEU	185	-1.182	-18.567	149.627	1.00	31.61	C	C
	ATOM	4618	CD1	LEU	185	-1.227	-20.085	149.532	1.00	29.87	C	C
	ATOM	4619	CD2	LEU	185	-2.076	-17.934	148.576	1.00	30.23	C	C
50	ATOM	4620	C	LEU	185	-2.142	-16.345	152.693	1.00	32.89	C	C
	ATOM	4621	O	LEU	185	-1.473	-16.343	153.723	1.00	32.68	C	O
	ATOM	4622	N	PRO	186	-3.455	-16.085	152.703	1.00	33.52	C	N
	ATOM	4623	CD	PRO	186	-4.404	-15.963	151.586	1.00	33.47	C	C
	ATOM	4624	CA	PRO	186	-4.110	-15.824	153.985	1.00	34.41	C	C
55	ATOM	4625	CB	PRO	186	-5.564	-15.552	153.588	1.00	34.21	C	C
	ATOM	4626	CG	PRO	186	-5.714	-16.243	152.264	1.00	34.41	C	C
	ATOM	4627	C	PRO	186	-3.952	-17.050	154.880	1.00	35.52	C	C
	ATOM	4628	O	PRO	186	-3.863	-18.176	154.389	1.00	35.54	C	O
	ATOM	4629	N	ILE	187	-3.907	-16.831	156.189	1.00	36.77	C	N
	ATOM	4630	CA	ILE	187	-3.728	-17.921	157.143	1.00	37.62	C	C
	ATOM	4631	CB	ILE	187	-3.844	-17.417	158.594	1.00	38.59	C	C
	ATOM	4632	CG2	ILE	187	-3.717	-18.588	159.562	1.00	39.09	C	C

-249-

5	ATOM	4633	CG1	ILE	187	-2.752	-16.381	158.871	1.00	39.17	C	C
	ATOM	4634	CD1	ILE	187	-1.337	-16.901	158.653	1.00	39.06	C	C
	ATOM	4635	C	ILE	187	-4.682	-19.092	156.964	1.00	37.72	C	C
	ATOM	4636	O	ILE	187	-4.264	-20.246	157.055	1.00	37.65	C	O
	ATOM	4637	N	GLU	188	-5.959	-18.808	156.717	1.00	37.53	C	N
10	ATOM	4638	CA	GLU	188	-6.939	-19.878	156.535	1.00	37.86	C	C
	ATOM	4639	CB	GLU	188	-8.341	-19.302	156.286	1.00	39.84	C	C
	ATOM	4640	CG	GLU	188	-8.424	-18.286	155.155	1.00	43.27	C	C
	ATOM	4641	CD	GLU	188	-8.379	-16.849	155.645	1.00	45.23	C	C
	ATOM	4642	OE1	GLU	188	-7.596	-16.550	156.578	1.00	45.96	C	O
15	ATOM	4643	OE2	GLU	188	-9.125	-16.015	155.084	1.00	46.68	C	O
	ATOM	4644	C	GLU	188	-6.558	-20.832	155.397	1.00	36.71	C	C
	ATOM	4645	O	GLU	188	-6.786	-22.041	155.487	1.00	35.74	C	O
	ATOM	4646	N	ASP	189	-5.977	-20.292	154.330	1.00	35.44	C	N
	ATOM	4647	CA	ASP	189	-5.563	-21.114	153.199	1.00	34.24	C	C
20	ATOM	4648	CB	ASP	189	-5.378	-20.255	151.946	1.00	35.42	C	C
	ATOM	4649	CG	ASP	189	-6.701	-19.753	151.380	1.00	36.94	C	C
	ATOM	4650	OD1	ASP	189	-6.722	-19.324	150.210	1.00	38.00	C	O
	ATOM	4651	OD2	ASP	189	-7.717	-19.781	152.105	1.00	38.31	C	O
	ATOM	4652	C	ASP	189	-4.279	-21.891	153.503	1.00	32.76	C	C
25	ATOM	4653	O	ASP	189	-4.089	-22.998	153.001	1.00	31.31	C	O
	ATOM	4654	N	GLN	190	-3.397	-21.311	154.313	1.00	31.50	C	N
	ATOM	4655	CA	GLN	190	-2.165	-21.995	154.694	1.00	31.34	C	C
	ATOM	4656	CB	GLN	190	-1.279	-21.090	155.565	1.00	31.81	C	C
	ATOM	4657	CG	GLN	190	-0.838	-19.803	154.884	1.00	32.88	C	C
30	ATOM	4658	CD	GLN	190	0.168	-19.006	155.699	1.00	33.88	C	C
	ATOM	4659	OE1	GLN	190	0.376	-17.816	155.452	1.00	35.31	C	O
	ATOM	4660	NE2	GLN	190	0.805	-19.658	156.663	1.00	32.82	C	N
	ATOM	4661	C	GLN	190	-2.569	-23.242	155.484	1.00	30.49	C	C
	ATOM	4662	O	GLN	190	-2.039	-24.326	155.258	1.00	29.34	C	O
35	ATOM	4663	N	ILE	191	-3.520	-23.070	156.402	1.00	30.50	C	N
	ATOM	4664	CA	ILE	191	-4.036	-24.163	157.227	1.00	30.60	C	C
	ATOM	4665	CB	ILE	191	-5.216	-23.701	158.133	1.00	31.67	C	C
	ATOM	4666	CG2	ILE	191	-5.683	-24.857	159.000	1.00	30.87	C	C
	ATOM	4667	CG1	ILE	191	-4.805	-22.512	159.006	1.00	32.04	C	C
40	ATOM	4668	CD1	ILE	191	-3.723	-22.813	159.995	1.00	33.57	C	C
	ATOM	4669	C	ILE	191	-4.574	-25.275	156.334	1.00	30.25	C	C
	ATOM	4670	O	ILE	191	-4.203	-26.445	156.476	1.00	29.94	C	O
	ATOM	4671	N	SER	192	-5.458	-24.899	155.415	1.00	28.90	C	N
	ATOM	4672	CA	SER	192	-6.075	-25.853	154.503	1.00	28.72	C	C
45	ATOM	4673	CB	SER	192	-7.119	-25.147	153.644	1.00	28.55	C	C
	ATOM	4674	OG	SER	192	-8.087	-24.534	154.472	1.00	31.09	C	O
	ATOM	4675	C	SER	192	-5.087	-26.587	153.605	1.00	27.78	C	C
	ATOM	4676	O	SER	192	-5.200	-27.797	153.420	1.00	27.73	C	O
	ATOM	4677	N	LEU	193	-4.129	-25.867	153.033	1.00	26.80	C	N
50	ATOM	4678	CA	LEU	193	-3.158	-26.519	152.168	1.00	26.77	C	C
	ATOM	4679	CB	LEU	193	-2.310	-25.489	151.415	1.00	26.32	C	C
	ATOM	4680	CG	LEU	193	-3.046	-24.625	150.384	1.00	26.16	C	C
	ATOM	4681	CD1	LEU	193	-2.009	-23.922	149.513	1.00	26.75	C	C
	ATOM	4682	CD2	LEU	193	-3.969	-25.479	149.519	1.00	24.72	C	C
55	ATOM	4683	C	LEU	193	-2.258	-27.469	152.952	1.00	26.50	C	C
	ATOM	4684	O	LEU	193	-1.932	-28.545	152.468	1.00	25.42	C	O
	ATOM	4685	N	LEU	194	-1.863	-27.074	154.159	1.00	26.75	C	N
	ATOM	4686	CA	LEU	194	-1.014	-27.925	154.991	1.00	27.59	C	C
	ATOM	4687	CB	LEU	194	-0.648	-27.222	156.301	1.00	28.17	C	C
	ATOM	4688	CG	LEU	194	0.163	-28.160	157.201	1.00	30.85	C	C
	ATOM	4689	CD1	LEU	194	1.636	-28.084	156.797	1.00	31.68	C	C
	ATOM	4690	CD2	LEU	194	-0.018	-27.795	158.662	1.00	32.14	C	C

-250-

5	ATOM	4691	C	LEU	194	-1.717	-29.246	155.323	1.00	27.29	C	C
	ATOM	4692	O	LEU	194	-1.151	-30.328	155.139	1.00	26.70	C	O
	ATOM	4693	N	LYS	195	-2.948	-29.148	155.818	1.00	26.53	C	N
	ATOM	4694	CA	LYS	195	-3.723	-30.327	156.172	1.00	27.06	C	C
	ATOM	4695	CB	LYS	195	-5.061	-29.918	156.803	1.00	28.79	C	C
	ATOM	4696	CG	LYS	195	-4.933	-29.205	158.138	1.00	31.86	C	C
	ATOM	4697	CD	LYS	195	-6.301	-28.898	158.740	1.00	34.00	C	C
10	ATOM	4698	CE	LYS	195	-6.164	-28.259	160.117	1.00	35.25	C	C
	ATOM	4699	NZ	LYS	195	-7.491	-28.066	160.781	1.00	37.11	C	N
	ATOM	4700	C	LYS	195	-3.988	-31.203	154.956	1.00	26.13	C	C
	ATOM	4701	O	LYS	195	-3.992	-32.430	155.048	1.00	26.21	C	O
15	ATOM	4702	N	GLY	196	-4.211	-30.572	153.812	1.00	24.83	C	N
	ATOM	4703	CA	GLY	196	-4.479	-31.327	152.606	1.00	23.63	C	C
	ATOM	4704	C	GLY	196	-3.286	-32.025	151.969	1.00	22.89	C	C
	ATOM	4705	O	GLY	196	-3.462	-33.047	151.306	1.00	21.84	C	O
	ATOM	4706	N	ALA	197	-2.076	-31.509	152.179	1.00	21.49	C	N
20	ATOM	4707	CA	ALA	197	-0.902	-32.105	151.545	1.00	21.24	C	C
	ATOM	4708	CB	ALA	197	-0.277	-31.082	150.584	1.00	19.64	C	C
	ATOM	4709	C	ALA	197	0.205	-32.708	152.421	1.00	20.04	C	C
	ATOM	4710	O	ALA	197	1.050	-33.433	151.905	1.00	19.54	C	O
	ATOM	4711	N	ALA	198	0.212	-32.411	153.717	1.00	18.80	C	N
25	ATOM	4712	CA	ALA	198	1.255	-32.915	154.616	1.00	17.78	C	C
	ATOM	4713	CB	ALA	198	0.868	-32.650	156.052	1.00	17.25	C	C
	ATOM	4714	C	ALA	198	1.632	-34.387	154.448	1.00	17.03	C	C
	ATOM	4715	O	ALA	198	2.811	-34.714	154.304	1.00	16.38	C	O
	ATOM	4716	N	VAL	199	0.648	-35.275	154.482	1.00	16.43	C	N
30	ATOM	4717	CA	VAL	199	0.927	-36.700	154.332	1.00	16.70	C	C
	ATOM	4718	CB	VAL	199	-0.328	-37.555	154.613	1.00	16.81	C	C
	ATOM	4719	CG1	VAL	199	-0.056	-39.021	154.262	1.00	17.35	C	C
	ATOM	4720	CG2	VAL	199	-0.707	-37.440	156.093	1.00	16.94	C	C
	ATOM	4721	C	VAL	199	1.458	-37.005	152.934	1.00	16.67	C	C
35	ATOM	4722	O	VAL	199	2.382	-37.802	152.778	1.00	15.71	C	O
	ATOM	4723	N	GLU	200	0.874	-36.375	151.920	1.00	16.31	C	N
	ATOM	4724	CA	GLU	200	1.325	-36.570	150.546	1.00	17.25	C	C
	ATOM	4725	CB	GLU	200	0.447	-35.762	149.589	1.00	18.45	C	C
	ATOM	4726	CG	GLU	200	-0.882	-36.426	149.242	1.00	19.72	C	C
40	ATOM	4727	CD	GLU	200	-1.770	-35.531	148.399	1.00	20.49	C	C
	ATOM	4728	OE1	GLU	200	-1.240	-34.820	147.526	1.00	20.99	C	O
	ATOM	4729	OE2	GLU	200	-2.999	-35.544	148.601	1.00	21.11	C	O
	ATOM	4730	C	GLU	200	2.796	-36.162	150.373	1.00	17.44	C	C
	ATOM	4731	O	GLU	200	3.596	-36.901	149.792	1.00	16.76	C	O
45	ATOM	4732	N	ILE	201	3.142	-34.980	150.875	1.00	17.66	C	N
	ATOM	4733	CA	ILE	201	4.507	-34.458	150.794	1.00	17.75	C	C
	ATOM	4734	CB	ILE	201	4.594	-33.045	151.458	1.00	18.15	C	C
	ATOM	4735	CG2	ILE	201	6.057	-32.649	151.706	1.00	17.40	C	C
	ATOM	4736	CG1	ILE	201	3.885	-32.018	150.561	1.00	17.68	C	C
50	ATOM	4737	CD1	ILE	201	3.686	-30.658	151.190	1.00	15.43	C	C
	ATOM	4738	C	ILE	201	5.468	-35.416	151.491	1.00	18.18	C	C
	ATOM	4739	O	ILE	201	6.542	-35.723	150.976	1.00	18.01	C	O
	ATOM	4740	N	CYS	202	5.077	-35.890	152.669	1.00	17.95	C	N
	ATOM	4741	CA	CYS	202	5.917	-36.812	153.417	1.00	18.27	C	C
55	ATOM	4742	CB	CYS	202	5.259	-37.161	154.752	1.00	17.78	C	C
	ATOM	4743	SG	CYS	202	5.370	-35.804	155.941	1.00	19.31	C	S
	ATOM	4744	C	CYS	202	6.239	-38.075	152.632	1.00	17.48	C	C
	ATOM	4745	O	CYS	202	7.365	-38.555	152.684	1.00	17.82	C	O
	ATOM	4746	N	HIS	203	5.266	-38.619	151.908	1.00	16.38	C	N
	ATOM	4747	CA	HIS	203	5.533	-39.818	151.121	1.00	16.70	C	C
	ATOM	4748	CB	HIS	203	4.229	-40.442	150.611	1.00	15.92	C	C

-251-

5	ATOM	4749	CG	HIS	203	3.524	-41.272	151.640	1.00	15.86	C	C
	ATOM	4750	CD2	HIS	203	2.354	-41.080	152.293	1.00	16.22	C	C
	ATOM	4751	ND1	HIS	203	4.057	-42.439	152.145	1.00	16.53	C	N
	ATOM	4752	CE1	HIS	203	3.246	-42.930	153.064	1.00	16.84	C	C
	ATOM	4753	NE2	HIS	203	2.205	-42.123	153.174	1.00	16.72	C	N
10	ATOM	4754	C	HIS	203	6.472	-39.519	149.962	1.00	16.55	C	C
	ATOM	4755	O	HIS	203	7.305	-40.352	149.601	1.00	17.66	C	O
	ATOM	4756	N	ILE	204	6.347	-38.331	149.378	1.00	16.27	C	N
	ATOM	4757	CA	ILE	204	7.219	-37.944	148.284	1.00	16.29	C	C
	ATOM	4758	CB	ILE	204	6.806	-36.571	147.704	1.00	16.08	C	C
15	ATOM	4759	CG2	ILE	204	7.903	-36.055	146.764	1.00	16.01	C	C
	ATOM	4760	CG1	ILE	204	5.469	-36.708	146.956	1.00	14.17	C	C
	ATOM	4761	CD1	ILE	204	4.892	-35.396	146.483	1.00	13.55	C	C
	ATOM	4762	C	ILE	204	8.664	-37.875	148.798	1.00	17.25	C	C
	ATOM	4763	O	ILE	204	9.586	-38.383	148.159	1.00	17.11	C	O
20	ATOM	4764	N	VAL	205	8.847	-37.248	149.956	1.00	17.08	C	N
	ATOM	4765	CA	VAL	205	10.159	-37.121	150.577	1.00	18.01	C	C
	ATOM	4766	CB	VAL	205	10.087	-36.200	151.819	1.00	17.13	C	C
	ATOM	4767	CG1	VAL	205	11.383	-36.276	152.608	1.00	16.96	C	C
	ATOM	4768	CG2	VAL	205	9.820	-34.765	151.372	1.00	16.00	C	C
25	ATOM	4769	C	VAL	205	10.711	-38.486	150.991	1.00	18.51	C	C
	ATOM	4770	O	VAL	205	11.887	-38.765	150.799	1.00	19.15	C	O
	ATOM	4771	N	LEU	206	9.859	-39.331	151.562	1.00	19.05	C	N
	ATOM	4772	CA	LEU	206	10.255	-40.671	151.993	1.00	20.76	C	C
	ATOM	4773	CB	LEU	206	9.140	-41.285	152.848	1.00	21.98	C	C
30	ATOM	4774	CG	LEU	206	9.329	-41.352	154.371	1.00	24.68	C	C
	ATOM	4775	CD1	LEU	206	10.072	-40.134	154.882	1.00	24.95	C	C
	ATOM	4776	CD2	LEU	206	7.964	-41.484	155.032	1.00	24.49	C	C
	ATOM	4777	C	LEU	206	10.590	-41.629	150.841	1.00	20.80	C	C
	ATOM	4778	O	LEU	206	11.225	-42.668	151.055	1.00	20.84	C	O
35	ATOM	4779	N	ASN	207	10.177	-41.292	149.623	1.00	19.96	C	N
	ATOM	4780	CA	ASN	207	10.442	-42.165	148.479	1.00	20.57	C	C
	ATOM	4781	CB	ASN	207	9.837	-41.573	147.199	1.00	18.23	C	C
	ATOM	4782	CG	ASN	207	9.915	-42.530	146.017	1.00	18.97	C	C
	ATOM	4783	OD1	ASN	207	10.590	-42.259	145.024	1.00	18.39	C	O
40	ATOM	4784	ND2	ASN	207	9.228	-43.656	146.123	1.00	16.71	C	N
	ATOM	4785	C	ASN	207	11.939	-42.452	148.280	1.00	20.94	C	C
	ATOM	4786	O	ASN	207	12.308	-43.563	147.885	1.00	20.03	C	O
	ATOM	4787	N	THR	208	12.797	-41.469	148.556	1.00	20.81	C	N
	ATOM	4788	CA	THR	208	14.235	-41.682	148.403	1.00	22.30	C	C
45	ATOM	4789	CB	THR	208	15.058	-40.375	148.528	1.00	22.75	C	C
	ATOM	4790	OG1	THR	208	14.576	-39.590	149.624	1.00	22.99	C	O
	ATOM	4791	CG2	THR	208	14.974	-39.583	147.239	1.00	25.40	C	C
	ATOM	4792	C	THR	208	14.811	-42.708	149.372	1.00	21.11	C	C
	ATOM	4793	O	THR	208	15.935	-43.148	149.190	1.00	21.58	C	O
50	ATOM	4794	N	THR	209	14.061	-43.095	150.400	1.00	20.44	C	N
	ATOM	4795	CA	THR	209	14.567	-44.120	151.308	1.00	20.16	C	C
	ATOM	4796	CB	THR	209	14.114	-43.896	152.773	1.00	21.00	C	C
	ATOM	4797	OG1	THR	209	12.733	-44.268	152.920	1.00	20.06	C	O
	ATOM	4798	CG2	THR	209	14.310	-42.427	153.178	1.00	19.21	C	C
55	ATOM	4799	C	THR	209	14.086	-45.511	150.869	1.00	20.37	C	C
	ATOM	4800	O	THR	209	14.535	-46.528	151.402	1.00	19.73	C	O
	ATOM	4801	N	PHE	210	13.190	-45.550	149.886	1.00	19.78	C	N
	ATOM	4802	CA	PHE	210	12.623	-46.803	149.404	1.00	21.06	C	C
	ATOM	4803	CB	PHE	210	11.379	-46.515	148.552	1.00	20.74	C	C
	ATOM	4804	CG	PHE	210	10.537	-47.728	148.271	1.00	20.23	C	C
	ATOM	4805	CD1	PHE	210	9.868	-48.381	149.303	1.00	20.70	C	C
	ATOM	4806	CD2	PHE	210	10.392	-48.204	146.969	1.00	19.93	C	C

-252-

5	ATOM	4807	CE1	PHE	210	9.062	-49.491	149.045	1.00	21.07	C	C
	ATOM	4808	CE2	PHE	210	9.592	-49.310	146.701	1.00	19.80	C	C
	ATOM	4809	CZ	PHE	210	8.924	-49.955	147.740	1.00	20.40	C	C
	ATOM	4810	C	PHE	210	13.605	-47.647	148.602	1.00	21.28	C	C
	ATOM	4811	O	PHE	210	14.202	-47.186	147.640	1.00	20.88	C	O
10	ATOM	4812	N	CYS	211	13.770	-48.892	149.015	1.00	22.28	C	N
	ATOM	4813	CA	CYS	211	14.670	-49.802	148.330	1.00	24.70	C	C
	ATOM	4814	CB	CYS	211	15.421	-50.656	149.352	1.00	25.33	C	C
	ATOM	4815	SG	CYS	211	16.567	-51.838	148.615	1.00	28.07	C	S
	ATOM	4816	C	CYS	211	13.834	-50.694	147.417	1.00	25.31	C	C
15	ATOM	4817	O	CYS	211	13.077	-51.533	147.889	1.00	24.53	C	O
	ATOM	4818	N	LEU	212	13.964	-50.502	146.111	1.00	26.95	C	N
	ATOM	4819	CA	LEU	212	13.206	-51.290	145.142	1.00	29.54	C	C
	ATOM	4820	CB	LEU	212	13.581	-50.859	143.724	1.00	29.30	C	C
	ATOM	4821	CG	LEU	212	13.098	-49.465	143.324	1.00	30.74	C	C
20	ATOM	4822	CD1	LEU	212	13.746	-49.044	142.004	1.00	30.10	C	C
	ATOM	4823	CD2	LEU	212	11.572	-49.475	143.211	1.00	28.92	C	C
	ATOM	4824	C	LEU	212	13.433	-52.795	145.298	1.00	30.81	C	C
	ATOM	4825	O	LEU	212	12.489	-53.587	145.277	1.00	30.78	C	O
	ATOM	4826	N	GLN	213	14.691	-53.176	145.469	1.00	31.69	C	N
25	ATOM	4827	CA	GLN	213	15.072	-54.571	145.616	1.00	33.12	C	C
	ATOM	4828	CB	GLN	213	16.594	-54.657	145.725	1.00	35.87	C	C
	ATOM	4829	CG	GLN	213	17.144	-56.046	145.991	1.00	39.28	C	C
	ATOM	4830	CD	GLN	213	18.662	-56.056	146.143	1.00	41.77	C	C
	ATOM	4831	OE1	GLN	213	19.260	-57.100	146.398	1.00	43.80	C	O
30	ATOM	4832	NE2	GLN	213	19.291	-54.890	145.985	1.00	43.06	C	N
	ATOM	4833	C	GLN	213	14.428	-55.310	146.792	1.00	32.23	C	C
	ATOM	4834	O	GLN	213	14.048	-56.474	146.667	1.00	32.37	C	O
	ATOM	4835	N	THR	214	14.288	-54.641	147.930	1.00	30.26	C	N
	ATOM	4836	CA	THR	214	13.720	-55.295	149.103	1.00	28.07	C	C
35	ATOM	4837	CB	THR	214	14.649	-55.133	150.331	1.00	28.29	C	C
	ATOM	4838	OG1	THR	214	14.781	-53.741	150.645	1.00	27.85	C	O
	ATOM	4839	CG2	THR	214	16.037	-55.711	150.047	1.00	28.08	C	C
	ATOM	4840	C	THR	214	12.336	-54.804	149.509	1.00	27.47	C	C
	ATOM	4841	O	THR	214	11.728	-55.366	150.420	1.00	26.07	C	O
40	ATOM	4842	N	GLN	215	11.842	-53.764	148.844	1.00	26.24	C	N
	ATOM	4843	CA	GLN	215	10.535	-53.196	149.175	1.00	27.14	C	C
	ATOM	4844	CB	GLN	215	9.433	-54.236	148.961	1.00	28.32	C	C
	ATOM	4845	CG	GLN	215	9.343	-54.776	147.533	1.00	32.89	C	C
	ATOM	4846	CD	GLN	215	8.932	-53.716	146.532	1.00	34.61	C	C
45	ATOM	4847	OE1	GLN	215	7.885	-53.085	146.676	1.00	36.92	C	O
	ATOM	4848	NE2	GLN	215	9.752	-53.517	145.509	1.00	35.80	C	N
	ATOM	4849	C	GLN	215	10.523	-52.715	150.639	1.00	25.79	C	C
	ATOM	4850	O	GLN	215	9.503	-52.779	151.318	1.00	25.44	C	O
	ATOM	4851	N	ASN	216	11.673	-52.240	151.103	1.00	24.70	C	N
50	ATOM	4852	CA	ASN	216	11.860	-51.738	152.467	1.00	24.04	C	C
	ATOM	4853	CB	ASN	216	13.101	-52.384	153.111	1.00	25.43	C	C
	ATOM	4854	CG	ASN	216	12.825	-53.730	153.744	1.00	28.21	C	C
	ATOM	4855	OD1	ASN	216	12.179	-54.595	153.156	1.00	28.27	C	O
	ATOM	4856	ND2	ASN	216	13.339	-53.919	154.958	1.00	30.94	C	N
55	ATOM	4857	C	ASN	216	12.143	-50.241	152.406	1.00	21.89	C	C
	ATOM	4858	O	ASN	216	12.680	-49.752	151.423	1.00	21.17	C	O
	ATOM	4859	N	PHE	217	11.790	-49.520	153.460	1.00	20.68	C	N
	ATOM	4860	CA	PHE	217	12.121	-48.100	153.538	1.00	20.49	C	C
	ATOM	4861	CB	PHE	217	10.989	-47.278	154.171	1.00	18.98	C	C
55	ATOM	4862	CG	PHE	217	9.809	-47.061	153.268	1.00	18.24	C	C
	ATOM	4863	CD1	PHE	217	8.778	-47.989	153.209	1.00	18.43	C	C
	ATOM	4864	CD2	PHE	217	9.728	-45.921	152.472	1.00	19.04	C	C

-253-

5	ATOM	4865	CE1	PHE	217	7.676	-47.783	152.366	1.00	20.17	C	C
	ATOM	4866	CE2	PHE	217	8.630	-45.706	151.622	1.00	18.75	C	C
	ATOM	4867	CZ	PHE	217	7.606	-46.636	151.571	1.00	18.41	C	C
	ATOM	4868	C	PHE	217	13.337	-48.103	154.472	1.00	20.87	C	C
	ATOM	4869	O	PHE	217	13.249	-48.577	155.602	1.00	19.76	C	O
10	ATOM	4870	N	LEU	218	14.466	-47.592	153.996	1.00	21.69	C	N
	ATOM	4871	CA	LEU	218	15.694	-47.560	154.790	1.00	22.93	C	C
	ATOM	4872	CB	LEU	218	16.895	-47.914	153.910	1.00	24.83	C	C
	ATOM	4873	CG	LEU	218	17.139	-49.352	153.445	1.00	26.67	C	C
	ATOM	4874	CD1	LEU	218	15.942	-49.895	152.686	1.00	28.70	C	C
15	ATOM	4875	CD2	LEU	218	18.375	-49.364	152.547	1.00	27.72	C	C
	ATOM	4876	C	LEU	218	15.922	-46.188	155.429	1.00	23.17	C	C
	ATOM	4877	O	LEU	218	16.311	-45.233	154.760	1.00	22.44	C	O
	ATOM	4878	N	CYS	219	15.700	-46.104	156.732	1.00	23.14	C	N
	ATOM	4879	CA	CYS	219	15.861	-44.843	157.435	1.00	24.43	C	C
20	ATOM	4880	CB	CYS	219	14.518	-44.436	158.052	1.00	23.99	C	C
	ATOM	4881	SG	CYS	219	13.158	-44.351	156.826	1.00	21.86	C	S
	ATOM	4882	C	CYS	219	16.945	-44.973	158.503	1.00	24.72	C	C
	ATOM	4883	O	CYS	219	16.666	-45.328	159.651	1.00	24.29	C	O
	ATOM	4884	N	GLY	220	18.181	-44.675	158.105	1.00	24.82	C	N
25	ATOM	4885	CA	GLY	220	19.305	-44.794	159.011	1.00	24.67	C	C
	ATOM	4886	C	GLY	220	19.418	-46.271	159.323	1.00	23.88	C	C
	ATOM	4887	O	GLY	220	19.472	-47.078	158.409	1.00	23.43	C	O
	ATOM	4888	N	PRO	221	19.456	-46.662	160.599	1.00	23.24	C	N
	ATOM	4889	CD	PRO	221	19.682	-45.837	161.801	1.00	23.12	C	C
30	ATOM	4890	CA	PRO	221	19.554	-48.092	160.913	1.00	22.65	C	C
	ATOM	4891	CB	PRO	221	20.239	-48.091	162.272	1.00	22.04	C	C
	ATOM	4892	CG	PRO	221	19.635	-46.863	162.926	1.00	21.62	C	C
	ATOM	4893	C	PRO	221	18.181	-48.785	160.964	1.00	22.50	C	C
	ATOM	4894	O	PRO	221	18.097	-49.971	161.265	1.00	22.01	C	O
35	ATOM	4895	N	LEU	222	17.111	-48.050	160.671	1.00	21.70	C	N
	ATOM	4896	CA	LEU	222	15.773	-48.625	160.721	1.00	21.85	C	C
	ATOM	4897	CB	LEU	222	14.795	-47.609	161.316	1.00	21.57	C	C
	ATOM	4898	CG	LEU	222	15.166	-47.060	162.700	1.00	20.39	C	C
	ATOM	4899	CD1	LEU	222	14.144	-46.021	163.131	1.00	20.86	C	C
40	ATOM	4900	CD2	LEU	222	15.229	-48.200	163.712	1.00	20.79	C	C
	ATOM	4901	C	LEU	222	15.258	-49.119	159.363	1.00	21.95	C	C
	ATOM	4902	O	LEU	222	15.582	-48.559	158.316	1.00	22.14	C	O
	ATOM	4903	N	ARG	223	14.449	-50.174	159.402	1.00	21.42	C	N
	ATOM	4904	CA	ARG	223	13.873	-50.768	158.198	1.00	21.84	C	C
45	ATOM	4905	CB	ARG	223	14.512	-52.133	157.921	1.00	23.26	C	C
	ATOM	4906	CG	ARG	223	16.038	-52.117	157.819	1.00	27.14	C	C
	ATOM	4907	CD	ARG	223	16.513	-51.551	156.482	1.00	30.23	C	C
	ATOM	4908	NE	ARG	223	17.977	-51.478	156.393	1.00	32.56	C	N
	ATOM	4909	CZ	ARG	223	18.721	-50.475	156.860	1.00	33.77	C	C
50	ATOM	4910	NH1	ARG	223	18.151	-49.435	157.455	1.00	31.71	C	N
	ATOM	4911	NH2	ARG	223	20.045	-50.510	156.728	1.00	35.18	C	N
	ATOM	4912	C	ARG	223	12.368	-50.955	158.381	1.00	20.01	C	C
	ATOM	4913	O	ARG	223	11.931	-51.654	159.290	1.00	20.43	C	O
	ATOM	4914	N	TYR	224	11.576	-50.335	157.517	1.00	17.42	C	N
55	ATOM	4915	CA	TYR	224	10.127	-50.468	157.599	1.00	15.88	C	C
	ATOM	4916	CB	TYR	224	9.442	-49.098	157.555	1.00	14.70	C	C
	ATOM	4917	CG	TYR	224	9.844	-48.159	158.674	1.00	15.19	C	C
	ATOM	4918	CD1	TYR	224	10.859	-47.221	158.488	1.00	14.65	C	C
	ATOM	4919	CE1	TYR	224	11.244	-46.359	159.514	1.00	15.25	C	C
55	ATOM	4920	CD2	TYR	224	9.219	-48.215	159.924	1.00	14.47	C	C
	ATOM	4921	CE2	TYR	224	9.601	-47.355	160.965	1.00	14.99	C	C
	ATOM	4922	CZ	TYR	224	10.615	-46.430	160.746	1.00	14.53	C	C

-254-

	ATOM	4923	OH	TYR	224	11.011	-45.570	161.740	1.00	13.71	C	O
	ATOM	4924	C	TYR	224	9.657	-51.312	156.420	1.00	15.26	C	C
	ATOM	4925	O	TYR	224	10.073	-51.087	155.290	1.00	12.96	C	O
5	ATOM	4926	N	THR	225	8.786	-52.277	156.693	1.00	14.87	C	N
	ATOM	4927	CA	THR	225	8.275	-53.162	155.647	1.00	15.88	C	C
	ATOM	4928	CB	THR	225	8.650	-54.639	155.919	1.00	15.32	C	C
	ATOM	4929	OG1	THR	225	8.026	-55.067	157.136	1.00	15.98	C	O
	ATOM	4930	CG2	THR	225	10.164	-54.799	156.045	1.00	15.24	C	C
10	ATOM	4931	C	THR	225	6.761	-53.068	155.592	1.00	14.70	C	C
	ATOM	4932	O	THR	225	6.150	-52.431	156.433	1.00	13.09	C	O
	ATOM	4933	N	ILE	226	6.160	-53.727	154.609	1.00	14.59	C	N
	ATOM	4934	CA	ILE	226	4.718	-53.695	154.465	1.00	14.58	C	C
	ATOM	4935	CB	ILE	226	4.288	-54.358	153.113	1.00	15.11	C	C
15	ATOM	4936	CG2	ILE	226	4.410	-55.877	153.183	1.00	12.89	C	C
	ATOM	4937	CG1	ILE	226	2.866	-53.929	152.746	1.00	14.93	C	C
	ATOM	4938	CD1	ILE	226	2.449	-54.325	151.320	1.00	14.79	C	C
	ATOM	4939	C	ILE	226	4.042	-54.347	155.678	1.00	15.04	C	C
	ATOM	4940	O	ILE	226	2.926	-53.970	156.046	1.00	14.65	C	O
20	ATOM	4941	N	GLU	227	4.727	-55.296	156.323	1.00	14.65	C	N
	ATOM	4942	CA	GLU	227	4.171	-55.955	157.506	1.00	15.12	C	C
	ATOM	4943	CB	GLU	227	5.091	-57.088	158.006	1.00	15.21	C	C
	ATOM	4944	CG	GLU	227	5.094	-58.390	157.162	1.00	17.13	C	C
	ATOM	4945	CD	GLU	227	5.727	-58.216	155.792	1.00	18.21	C	C
25	ATOM	4946	OE1	GLU	227	6.763	-57.530	155.700	1.00	20.90	C	O
	ATOM	4947	OE2	GLU	227	5.202	-58.763	154.804	1.00	18.86	C	O
	ATOM	4948	C	GLU	227	3.938	-54.965	158.654	1.00	14.83	C	C
	ATOM	4949	O	GLU	227	3.057	-55.178	159.487	1.00	14.73	C	O
	ATOM	4950	N	ASP	228	4.724	-53.893	158.717	1.00	14.22	C	N
30	ATOM	4951	CA	ASP	228	4.539	-52.923	159.793	1.00	15.26	C	C
	ATOM	4952	CB	ASP	228	5.684	-51.899	159.807	1.00	14.81	C	C
	ATOM	4953	CG	ASP	228	7.035	-52.548	160.109	1.00	16.58	C	C
	ATOM	4954	OD1	ASP	228	7.097	-53.348	161.069	1.00	15.48	C	O
	ATOM	4955	OD2	ASP	228	8.026	-52.269	159.391	1.00	15.15	C	O
35	ATOM	4956	C	ASP	228	3.186	-52.238	159.636	1.00	15.16	C	C
	ATOM	4957	O	ASP	228	2.456	-52.046	160.609	1.00	15.37	C	O
	ATOM	4958	N	GLY	229	2.846	-51.890	158.400	1.00	15.16	C	N
	ATOM	4959	CA	GLY	229	1.567	-51.258	158.151	1.00	14.56	C	C
	ATOM	4960	C	GLY	229	0.434	-52.235	158.416	1.00	14.33	C	C
40	ATOM	4961	O	GLY	229	-0.597	-51.870	158.987	1.00	12.80	C	O
	ATOM	4962	N	ALA	230	0.623	-53.492	158.023	1.00	13.05	C	N
	ATOM	4963	CA	ALA	230	-0.428	-54.479	158.223	1.00	13.45	C	C
	ATOM	4964	CB	ALA	230	-0.109	-55.753	157.452	1.00	12.06	C	C
	ATOM	4965	C	ALA	230	-0.657	-54.792	159.701	1.00	13.54	C	C
45	ATOM	4966	O	ALA	230	-1.804	-54.950	160.131	1.00	12.94	C	O
	ATOM	4967	N	ARG	231	0.420	-54.871	160.482	1.00	13.80	C	N
	ATOM	4968	CA	ARG	231	0.287	-55.179	161.903	1.00	14.40	C	C
	ATOM	4969	CB	ARG	231	1.653	-55.534	162.536	1.00	15.07	C	C
	ATOM	4970	CG	ARG	231	2.326	-56.828	162.018	1.00	16.54	C	C
	ATOM	4971	CD	ARG	231	1.472	-58.091	162.238	1.00	16.33	C	C
50	ATOM	4972	NE	ARG	231	1.410	-58.535	163.632	1.00	16.45	C	N
	ATOM	4973	CZ	ARG	231	2.348	-59.254	164.250	1.00	17.78	C	C
	ATOM	4974	NH1	ARG	231	3.448	-59.625	163.611	1.00	17.87	C	N
	ATOM	4975	NH2	ARG	231	2.176	-59.623	165.514	1.00	18.04	C	N
	ATOM	4976	C	ARG	231	-0.380	-54.056	162.710	1.00	14.96	C	C
55	ATOM	4977	O	ARG	231	-0.881	-54.312	163.797	1.00	14.90	C	O
	ATOM	4978	N	VAL	232	-0.383	-52.818	162.207	1.00	15.16	C	N
	ATOM	4979	CA	VAL	232	-1.044	-51.741	162.949	1.00	15.82	C	C
	ATOM	4980	CB	VAL	232	-0.277	-50.372	162.862	1.00	15.90	C	C

-255-

5	ATOM	4981	CG1	VAL	232	1.126	-50.538	163.444	1.00	15.46	C	C
	ATOM	4982	CG2	VAL	232	-0.222	-49.852	161.421	1.00	13.24	C	C
	ATOM	4983	C	VAL	232	-2.496	-51.562	162.503	1.00	15.62	C	C
	ATOM	4984	O	VAL	232	-3.213	-50.718	163.033	1.00	14.53	C	O
	ATOM	4985	N	GLY	233	-2.937	-52.367	161.535	1.00	16.24	C	N
10	ATOM	4986	CA	GLY	233	-4.324	-52.284	161.104	1.00	17.01	C	C
	ATOM	4987	C	GLY	233	-4.671	-51.859	159.687	1.00	17.97	C	C
	ATOM	4988	O	GLY	233	-5.846	-51.926	159.299	1.00	18.13	C	O
	ATOM	4989	N	PHE	234	-3.694	-51.411	158.904	1.00	17.03	C	N
	ATOM	4990	CA	PHE	234	-4.002	-51.016	157.539	1.00	17.34	C	C
15	ATOM	4991	CB	PHE	234	-2.817	-50.295	156.897	1.00	17.03	C	C
	ATOM	4992	CG	PHE	234	-2.602	-48.908	157.421	1.00	18.50	C	C
	ATOM	4993	CD1	PHE	234	-1.481	-48.605	158.197	1.00	17.96	C	C
	ATOM	4994	CD2	PHE	234	-3.524	-47.899	157.137	1.00	17.72	C	C
	ATOM	4995	CE1	PHE	234	-1.278	-47.310	158.684	1.00	19.80	C	C
20	ATOM	4996	CE2	PHE	234	-3.337	-46.604	157.616	1.00	18.38	C	C
	ATOM	4997	CZ	PHE	234	-2.207	-46.306	158.393	1.00	20.51	C	C
	ATOM	4998	C	PHE	234	-4.370	-52.235	156.703	1.00	18.19	C	C
	ATOM	4999	O	PHE	234	-3.834	-53.328	156.909	1.00	17.65	C	O
	ATOM	5000	N	GLN	235	-5.298	-52.046	155.767	1.00	18.33	C	N
25	ATOM	5001	CA	GLN	235	-5.728	-53.121	154.888	1.00	19.22	C	C
	ATOM	5002	CB	GLN	235	-7.036	-52.743	154.184	1.00	19.75	C	C
	ATOM	5003	CG	GLN	235	-8.206	-52.566	155.144	1.00	21.43	C	C
	ATOM	5004	CD	GLN	235	-9.519	-52.313	154.432	1.00	22.69	C	C
	ATOM	5005	OE1	GLN	235	-9.633	-51.402	153.608	1.00	22.47	C	O
30	ATOM	5006	NE2	GLN	235	-10.521	-53.118	154.751	1.00	22.23	C	N
	ATOM	5007	C	GLN	235	-4.637	-53.398	153.864	1.00	19.00	C	C
	ATOM	5008	O	GLN	235	-3.959	-52.486	153.393	1.00	17.75	C	O
	ATOM	5009	N	VAL	236	-4.472	-54.665	153.515	1.00	19.65	C	N
	ATOM	5010	CA	VAL	236	-3.440	-55.045	152.564	1.00	19.44	C	C
35	ATOM	5011	CB	VAL	236	-3.408	-56.565	152.354	1.00	19.19	C	C
	ATOM	5012	CG1	VAL	236	-2.335	-56.927	151.320	1.00	17.93	C	C
	ATOM	5013	CG2	VAL	236	-3.127	-57.247	153.681	1.00	18.12	C	C
	ATOM	5014	C	VAL	236	-3.561	-54.360	151.218	1.00	19.53	C	C
	ATOM	5015	O	VAL	236	-2.554	-53.943	150.648	1.00	18.39	C	O
40	ATOM	5016	N	GLU	237	-4.784	-54.251	150.708	1.00	19.52	C	N
	ATOM	5017	CA	GLU	237	-5.021	-53.598	149.418	1.00	20.17	C	C
	ATOM	5018	CB	GLU	237	-6.512	-53.631	149.088	1.00	22.85	C	C
	ATOM	5019	CG	GLU	237	-6.863	-53.098	147.717	1.00	27.72	C	C
	ATOM	5020	CD	GLU	237	-8.353	-53.206	147.431	1.00	31.75	C	C
45	ATOM	5021	OE1	GLU	237	-9.154	-52.737	148.270	1.00	33.80	C	O
	ATOM	5022	OE2	GLU	237	-8.723	-53.757	146.371	1.00	33.68	C	O
	ATOM	5023	C	GLU	237	-4.518	-52.148	149.454	1.00	18.07	C	C
	ATOM	5024	O	GLU	237	-3.840	-51.695	148.534	1.00	16.31	C	O
	ATOM	5025	N	PHE	238	-4.863	-51.427	150.515	1.00	16.98	C	N
50	ATOM	5026	CA	PHE	238	-4.400	-50.050	150.693	1.00	17.27	C	C
	ATOM	5027	CB	PHE	238	-4.910	-49.485	152.027	1.00	17.34	C	C
	ATOM	5028	CG	PHE	238	-4.299	-48.167	152.397	1.00	17.96	C	C
	ATOM	5029	CD1	PHE	238	-4.625	-47.007	151.694	1.00	18.18	C	C
	ATOM	5030	CD2	PHE	238	-3.363	-48.087	153.421	1.00	18.28	C	C
55	ATOM	5031	CE1	PHE	238	-4.023	-45.790	152.006	1.00	17.80	C	C
	ATOM	5032	CE2	PHE	238	-2.754	-46.872	153.743	1.00	18.89	C	C
	ATOM	5033	CZ	PHE	238	-3.085	-45.721	153.032	1.00	18.33	C	C
	ATOM	5034	C	PHE	238	-2.863	-50.058	150.703	1.00	16.70	C	C
	ATOM	5035	O	PHE	238	-2.215	-49.278	150.008	1.00	16.30	C	O
	ATOM	5036	N	LEU	239	-2.290	-50.951	151.505	1.00	16.06	C	N
	ATOM	5037	CA	LEU	239	-0.841	-51.080	151.615	1.00	17.40	C	C
	ATOM	5038	CB	LEU	239	-0.502	-52.212	152.598	1.00	15.80	C	C

-256-

5	ATOM	5039	CG	LEU	239	-0.056	-51.903	154.046	1.00	17.46	C	C
	ATOM	5040	CD1	LEU	239	-0.442	-50.502	154.480	1.00	15.39	C	C
	ATOM	5041	CD2	LEU	239	-0.643	-52.946	154.982	1.00	16.59	C	C
	ATOM	5042	C	LEU	239	-0.192	-51.335	150.246	1.00	17.56	C	C
	ATOM	5043	O	LEU	239	0.800	-50.696	149.902	1.00	17.19	C	O
10	ATOM	5044	N	GLU	240	-0.757	-52.257	149.468	1.00	18.40	C	N
	ATOM	5045	CA	GLU	240	-0.230	-52.585	148.145	1.00	20.85	C	C
	ATOM	5046	CB	GLU	240	-1.014	-53.752	147.521	1.00	23.02	C	C
	ATOM	5047	CG	GLU	240	-0.852	-55.083	148.259	1.00	26.39	C	C
	ATOM	5048	CD	GLU	240	0.483	-55.778	147.972	1.00	30.97	C	C
15	ATOM	5049	OE1	GLU	240	1.511	-55.087	147.772	1.00	32.51	C	O
	ATOM	5050	OE2	GLU	240	0.509	-57.028	147.958	1.00	33.15	C	O
	ATOM	5051	C	GLU	240	-0.289	-51.366	147.230	1.00	20.90	C	C
	ATOM	5052	O	GLU	240	0.632	-51.126	146.454	1.00	20.74	C	O
	ATOM	5053	N	LEU	241	-1.369	-50.596	147.316	1.00	21.07	C	N
20	ATOM	5054	CA	LEU	241	-1.490	-49.391	146.501	1.00	22.58	C	C
	ATOM	5055	CB	LEU	241	-2.837	-48.705	146.741	1.00	24.26	C	C
	ATOM	5056	CG	LEU	241	-2.977	-47.320	146.093	1.00	26.53	C	C
	ATOM	5057	CD1	LEU	241	-2.920	-47.448	144.575	1.00	27.75	C	C
	ATOM	5058	CD2	LEU	241	-4.295	-46.683	146.513	1.00	28.98	C	C
25	ATOM	5059	C	LEU	241	-0.369	-48.416	146.865	1.00	22.18	C	C
	ATOM	5060	O	LEU	241	0.233	-47.790	145.997	1.00	22.71	C	O
	ATOM	5061	N	LEU	242	-0.088	-48.301	148.158	1.00	20.92	C	N
	ATOM	5062	CA	LEU	242	0.946	-47.400	148.628	1.00	20.02	C	C
	ATOM	5063	CB	LEU	242	0.860	-47.274	150.153	1.00	20.07	C	C
30	ATOM	5064	CG	LEU	242	1.789	-46.252	150.806	1.00	21.59	C	C
	ATOM	5065	CD1	LEU	242	1.568	-44.864	150.189	1.00	20.97	C	C
	ATOM	5066	CD2	LEU	242	1.520	-46.231	152.299	1.00	19.92	C	C
	ATOM	5067	C	LEU	242	2.345	-47.840	148.196	1.00	19.08	C	C
	ATOM	5068	O	LEU	242	3.118	-47.039	147.680	1.00	18.08	C	O
35	ATOM	5069	N	PHE	243	2.673	-49.110	148.396	1.00	18.57	C	N
	ATOM	5070	CA	PHE	243	3.990	-49.601	148.006	1.00	18.80	C	C
	ATOM	5071	CB	PHE	243	4.243	-50.992	148.603	1.00	16.93	C	C
	ATOM	5072	CG	PHE	243	4.694	-50.958	150.053	1.00	15.95	C	C
	ATOM	5073	CD1	PHE	243	3.861	-50.446	151.049	1.00	15.49	C	C
40	ATOM	5074	CD2	PHE	243	5.962	-51.407	150.410	1.00	14.54	C	C
	ATOM	5075	CE1	PHE	243	4.283	-50.377	152.384	1.00	15.83	C	C
	ATOM	5076	CE2	PHE	243	6.400	-51.345	151.738	1.00	15.46	C	C
	ATOM	5077	CZ	PHE	243	5.557	-50.827	152.732	1.00	14.97	C	C
	ATOM	5078	C	PHE	243	4.198	-49.603	146.484	1.00	19.80	C	C
45	ATOM	5079	O	PHE	243	5.320	-49.407	146.010	1.00	18.39	C	O
	ATOM	5080	N	HIS	244	3.126	-49.807	145.720	1.00	20.82	C	N
	ATOM	5081	CA	HIS	244	3.230	-49.786	144.258	1.00	22.43	C	C
	ATOM	5082	CB	HIS	244	1.921	-50.256	143.609	1.00	25.14	C	C
	ATOM	5083	CG	HIS	244	1.973	-50.310	142.112	1.00	29.07	C	C
50	ATOM	5084	CD2	HIS	244	2.463	-51.251	141.269	1.00	30.07	C	C
	ATOM	5085	ND1	HIS	244	1.499	-49.291	141.312	1.00	29.94	C	N
	ATOM	5086	CE1	HIS	244	1.692	-49.603	140.042	1.00	30.15	C	C
	ATOM	5087	NE2	HIS	244	2.276	-50.787	139.989	1.00	30.65	C	N
	ATOM	5088	C	HIS	244	3.549	-48.353	143.834	1.00	21.93	C	C
55	ATOM	5089	O	HIS	244	4.334	-48.125	142.914	1.00	21.81	C	O
	ATOM	5090	N	PHE	245	2.927	-47.389	144.510	1.00	20.16	C	N
	ATOM	5091	CA	PHE	245	3.187	-45.986	144.240	1.00	19.29	C	C
	ATOM	5092	CB	PHE	245	2.377	-45.097	145.195	1.00	19.02	C	C
	ATOM	5093	CG	PHE	245	2.844	-43.667	145.238	1.00	18.10	C	C
	ATOM	5094	CD1	PHE	245	2.475	-42.767	144.242	1.00	18.27	C	C
	ATOM	5095	CD2	PHE	245	3.679	-43.228	146.263	1.00	18.82	C	C
	ATOM	5096	CE1	PHE	245	2.928	-41.451	144.264	1.00	18.07	C	C

-257-

5	ATOM	5097	CE2	PHE	245	4.142	-41.913	146.300	1.00	18.71	C	C
	ATOM	5098	CZ	PHE	245	3.764	-41.020	145.295	1.00	19.85	C	C
	ATOM	5099	C	PHE	245	4.675	-45.727	144.470	1.00	18.96	C	C
	ATOM	5100	O	PHE	245	5.355	-45.156	143.621	1.00	17.49	C	O
	ATOM	5101	N	HIS	246	5.175	-46.138	145.633	1.00	17.92	C	N
10	ATOM	5102	CA	HIS	246	6.577	-45.917	145.948	1.00	18.17	C	C
	ATOM	5103	CB	HIS	246	6.872	-46.353	147.382	1.00	17.39	C	C
	ATOM	5104	CG	HIS	246	6.504	-45.318	148.402	1.00	16.79	C	C
	ATOM	5105	CD2	HIS	246	5.474	-45.253	149.279	1.00	16.89	C	C
	ATOM	5106	ND1	HIS	246	7.211	-44.145	148.555	1.00	14.73	C	N
15	ATOM	5107	CE1	HIS	246	6.631	-43.400	149.480	1.00	16.89	C	C
	ATOM	5108	NE2	HIS	246	5.574	-44.050	149.936	1.00	16.76	C	N
	ATOM	5109	C	HIS	246	7.533	-46.576	144.962	1.00	17.97	C	C
	ATOM	5110	O	HIS	246	8.511	-45.968	144.560	1.00	17.61	C	O
	ATOM	5111	N	GLY	247	7.243	-47.803	144.552	1.00	18.68	C	N
20	ATOM	5112	CA	GLY	247	8.106	-48.462	143.587	1.00	19.53	C	C
	ATOM	5113	C	GLY	247	8.106	-47.744	142.243	1.00	20.19	C	C
	ATOM	5114	O	GLY	247	9.160	-47.522	141.646	1.00	20.80	C	O
	ATOM	5115	N	THR	248	6.921	-47.373	141.765	1.00	19.87	C	N
	ATOM	5116	CA	THR	248	6.778	-46.677	140.491	1.00	19.32	C	C
25	ATOM	5117	CB	THR	248	5.281	-46.434	140.160	1.00	19.66	C	C
	ATOM	5118	OG1	THR	248	4.577	-47.682	140.176	1.00	19.35	C	O
	ATOM	5119	CG2	THR	248	5.127	-45.814	138.783	1.00	18.52	C	C
	ATOM	5120	C	THR	248	7.519	-45.335	140.491	1.00	19.29	C	C
	ATOM	5121	O	THR	248	8.259	-45.029	139.554	1.00	18.25	C	O
30	ATOM	5122	N	LEU	249	7.320	-44.530	141.531	1.00	18.21	C	N
	ATOM	5123	CA	LEU	249	7.999	-43.238	141.604	1.00	19.06	C	C
	ATOM	5124	CB	LEU	249	7.520	-42.446	142.826	1.00	18.37	C	C
	ATOM	5125	CG	LEU	249	8.207	-41.096	143.067	1.00	19.31	C	C
	ATOM	5126	CD1	LEU	249	7.956	-40.168	141.886	1.00	17.37	C	C
35	ATOM	5127	CD2	LEU	249	7.677	-40.468	144.356	1.00	19.95	C	C
	ATOM	5128	C	LEU	249	9.518	-43.428	141.694	1.00	19.08	C	C
	ATOM	5129	O	LEU	249	10.278	-42.760	140.998	1.00	18.35	C	O
	ATOM	5130	N	ARG	250	9.949	-44.342	142.555	1.00	19.05	C	N
	ATOM	5131	CA	ARG	250	11.370	-44.605	142.748	1.00	21.51	C	C
40	ATOM	5132	CB	ARG	250	11.560	-45.712	143.793	1.00	22.24	C	C
	ATOM	5133	CG	ARG	250	13.002	-45.878	144.286	1.00	25.15	C	C
	ATOM	5134	CD	ARG	250	13.451	-44.658	145.095	1.00	27.57	C	C
	ATOM	5135	NE	ARG	250	14.457	-45.005	146.097	1.00	29.42	C	N
	ATOM	5136	CZ	ARG	250	15.772	-44.954	145.909	1.00	31.82	C	C
45	ATOM	5137	NH1	ARG	250	16.272	-44.559	144.747	1.00	33.24	C	N
	ATOM	5138	NH2	ARG	250	16.594	-45.318	146.884	1.00	32.37	C	N
	ATOM	5139	C	ARG	250	12.069	-45.016	141.448	1.00	22.35	C	C
	ATOM	5140	O	ARG	250	13.192	-44.592	141.182	1.00	21.30	C	O
	ATOM	5141	N	LYS	251	11.396	-45.835	140.640	1.00	23.28	C	N
50	ATOM	5142	CA	LYS	251	11.973	-46.311	139.385	1.00	24.95	C	C
	ATOM	5143	CB	LYS	251	11.072	-47.375	138.750	1.00	25.59	C	C
	ATOM	5144	CG	LYS	251	11.096	-48.727	139.454	1.00	27.12	C	C
	ATOM	5145	CD	LYS	251	10.179	-49.729	138.759	1.00	29.13	C	C
	ATOM	5146	CE	LYS	251	9.952	-50.967	139.620	1.00	30.83	C	C
55	ATOM	5147	NZ	LYS	251	8.907	-51.877	139.064	1.00	31.97	C	N
	ATOM	5148	C	LYS	251	12.262	-45.222	138.359	1.00	25.23	C	C
	ATOM	5149	O	LYS	251	13.053	-45.437	137.439	1.00	25.25	C	O
	ATOM	5150	N	LEU	252	11.631	-44.059	138.511	1.00	24.72	C	N
	ATOM	5151	CA	LEU	252	11.843	-42.960	137.577	1.00	25.19	C	C
55	ATOM	5152	CB	LEU	252	10.683	-41.966	137.668	1.00	24.25	C	C
	ATOM	5153	CG	LEU	252	9.307	-42.516	137.278	1.00	25.10	C	C
	ATOM	5154	CD1	LEU	252	8.227	-41.491	137.611	1.00	24.20	C	C

-258-

5	ATOM	5155	CD2	LEU	252	9.287	-42.861	135.783	1.00	24.17	C	C
	ATOM	5156	C	LEU	252	13.174	-42.232	137.792	1.00	26.15	C	C
	ATOM	5157	O	LEU	252	13.537	-41.354	137.013	1.00	26.54	C	O
	ATOM	5158	N	GLN	253	13.894	-42.591	138.852	1.00	27.14	C	N
10	ATOM	5159	CA	GLN	253	15.182	-41.979	139.147	1.00	28.03	C	C
	ATOM	5160	CB	GLN	253	16.236	-42.492	138.159	1.00	29.58	C	C
	ATOM	5161	CG	GLN	253	16.524	-43.989	138.273	1.00	31.02	C	C
	ATOM	5162	CD	GLN	253	17.517	-44.495	137.228	1.00	33.14	C	C
15	ATOM	5163	OE1	GLN	253	17.954	-45.643	137.286	1.00	35.27	C	O
	ATOM	5164	NE2	GLN	253	17.869	-43.644	136.266	1.00	33.37	C	N
	ATOM	5165	C	GLN	253	15.113	-40.461	139.074	1.00	27.47	C	C
	ATOM	5166	O	GLN	253	15.838	-39.836	138.308	1.00	27.66	C	O
20	ATOM	5167	N	LEU	254	14.241	-39.870	139.876	1.00	27.11	C	N
	ATOM	5168	CA	LEU	254	14.091	-38.428	139.881	1.00	26.74	C	C
	ATOM	5169	CB	LEU	254	12.811	-38.018	140.623	1.00	25.22	C	C
	ATOM	5170	CG	LEU	254	11.452	-38.440	140.051	1.00	24.23	C	C
25	ATOM	5171	CD1	LEU	254	10.345	-37.659	140.762	1.00	22.94	C	C
	ATOM	5172	CD2	LEU	254	11.402	-38.170	138.557	1.00	22.58	C	C
	ATOM	5173	C	LEU	254	15.278	-37.734	140.528	1.00	27.44	C	C
	ATOM	5174	O	LEU	254	15.953	-38.288	141.395	1.00	26.90	C	O
30	ATOM	5175	N	GLN	255	15.535	-36.519	140.075	1.00	28.34	C	N
	ATOM	5176	CA	GLN	255	16.601	-35.708	140.625	1.00	30.41	C	C
	ATOM	5177	CB	GLN	255	17.169	-34.796	139.542	1.00	32.70	C	C
	ATOM	5178	CG	GLN	255	18.036	-35.532	138.521	1.00	35.87	C	C
35	ATOM	5179	CD	GLN	255	18.246	-34.728	137.255	1.00	37.99	C	C
	ATOM	5180	OE1	GLN	255	18.427	-33.510	137.303	1.00	39.69	C	O
	ATOM	5181	NE2	GLN	255	18.226	-35.404	136.111	1.00	39.40	C	N
	ATOM	5182	C	GLN	255	15.930	-34.896	141.726	1.00	30.12	C	C
40	ATOM	5183	O	GLN	255	14.709	-34.752	141.732	1.00	29.99	C	O
	ATOM	5184	N	GLU	256	16.711	-34.371	142.658	1.00	30.10	C	N
	ATOM	5185	CA	GLU	256	16.136	-33.613	143.757	1.00	30.45	C	C
	ATOM	5186	CB	GLU	256	17.245	-33.047	144.646	1.00	32.12	C	C
45	ATOM	5187	CG	GLU	256	16.720	-32.478	145.946	1.00	35.72	C	C
	ATOM	5188	CD	GLU	256	17.820	-32.173	146.936	1.00	37.90	C	C
	ATOM	5189	OE1	GLU	256	18.624	-31.249	146.676	1.00	39.48	C	O
	ATOM	5190	OE2	GLU	256	17.881	-32.867	147.973	1.00	39.28	C	O
50	ATOM	5191	C	GLU	256	15.166	-32.494	143.354	1.00	29.53	C	C
	ATOM	5192	O	GLU	256	14.093	-32.364	143.946	1.00	28.88	C	O
	ATOM	5193	N	PRO	257	15.521	-31.668	142.349	1.00	28.61	C	N
	ATOM	5194	CD	PRO	257	16.778	-31.542	141.589	1.00	28.20	C	C
55	ATOM	5195	CA	PRO	257	14.584	-30.603	141.976	1.00	27.69	C	C
	ATOM	5196	CB	PRO	257	15.295	-29.905	140.820	1.00	27.66	C	C
	ATOM	5197	CG	PRO	257	16.744	-30.090	141.169	1.00	28.71	C	C
	ATOM	5198	C	PRO	257	13.213	-31.141	141.570	1.00	26.87	C	C
55	ATOM	5199	O	PRO	257	12.187	-30.550	141.891	1.00	26.59	C	O
	ATOM	5200	N	GLU	258	13.199	-32.261	140.858	1.00	25.85	C	N
	ATOM	5201	CA	GLU	258	11.940	-32.859	140.418	1.00	24.88	C	C
	ATOM	5202	CB	GLU	258	12.222	-34.005	139.439	1.00	24.17	C	C
55	ATOM	5203	CG	GLU	258	12.986	-33.528	138.205	1.00	25.10	C	C
	ATOM	5204	CD	GLU	258	13.541	-34.659	137.360	1.00	26.23	C	C
	ATOM	5205	OE1	GLU	258	14.026	-35.661	137.933	1.00	25.87	C	O
	ATOM	5206	OE2	GLU	258	13.515	-34.533	136.118	1.00	27.53	C	O
55	ATOM	5207	C	GLU	258	11.140	-33.341	141.629	1.00	23.84	C	C
	ATOM	5208	O	GLU	258	9.921	-33.177	141.678	1.00	22.84	C	O
	ATOM	5209	N	TYR	259	11.831	-33.911	142.611	1.00	22.35	C	N
	ATOM	5210	CA	TYR	259	11.176	-34.376	143.827	1.00	22.61	C	C
55	ATOM	5211	CB	TYR	259	12.177	-35.073	144.760	1.00	21.98	C	C
	ATOM	5212	CG	TYR	259	12.258	-36.588	144.617	1.00	21.14	C	C

-259-

5	ATOM	5213	CD1	TYR	259	11.120	-37.395	144.761	1.00	20.56	C	C
	ATOM	5214	CE1	TYR	259	11.206	-38.794	144.691	1.00	18.62	C	C
	ATOM	5215	CD2	TYR	259	13.481	-37.217	144.394	1.00	20.34	C	C
	ATOM	5216	CE2	TYR	259	13.581	-38.607	144.320	1.00	19.30	C	C
	ATOM	5217	CZ	TYR	259	12.443	-39.389	144.473	1.00	19.88	C	C
10	ATOM	5218	OH	TYR	259	12.564	-40.761	144.427	1.00	17.21	C	O
	ATOM	5219	C	TYR	259	10.523	-33.217	144.582	1.00	22.27	C	C
	ATOM	5220	O	TYR	259	9.348	-33.298	144.944	1.00	21.25	C	O
	ATOM	5221	N	VAL	260	11.267	-32.132	144.805	1.00	21.69	C	N
	ATOM	5222	CA	VAL	260	10.710	-31.007	145.551	1.00	21.85	C	C
15	ATOM	5223	CB	VAL	260	11.807	-29.997	146.028	1.00	21.84	C	C
	ATOM	5224	CG1	VAL	260	12.886	-30.741	146.804	1.00	23.44	C	C
	ATOM	5225	CG2	VAL	260	12.400	-29.245	144.853	1.00	21.89	C	C
	ATOM	5226	C	VAL	260	9.643	-30.256	144.779	1.00	21.44	C	C
	ATOM	5227	O	VAL	260	8.731	-29.681	145.376	1.00	19.91	C	O
20	ATOM	5228	N	LEU	261	9.758	-30.257	143.456	1.00	21.26	C	N
	ATOM	5229	CA	LEU	261	8.782	-29.579	142.609	1.00	23.04	C	C
	ATOM	5230	CB	LEU	261	9.309	-29.508	141.172	1.00	24.60	C	C
	ATOM	5231	CG	LEU	261	9.510	-28.172	140.440	1.00	24.84	C	C
	ATOM	5232	CD1	LEU	261	9.586	-27.008	141.388	1.00	24.16	C	C
25	ATOM	5233	CD2	LEU	261	10.784	-28.282	139.599	1.00	25.17	C	C
	ATOM	5234	C	LEU	261	7.481	-30.377	142.667	1.00	22.74	C	C
	ATOM	5235	O	LEU	261	6.394	-29.818	142.611	1.00	22.54	C	O
	ATOM	5236	N	LEU	262	7.612	-31.694	142.792	1.00	23.07	C	N
	ATOM	5237	CA	LEU	262	6.464	-32.587	142.887	1.00	23.17	C	C
30	ATOM	5238	CB	LEU	262	6.950	-34.033	142.863	1.00	24.16	C	C
	ATOM	5239	CG	LEU	262	5.954	-35.134	142.507	1.00	27.12	C	C
	ATOM	5240	CD1	LEU	262	5.333	-34.850	141.135	1.00	26.19	C	C
	ATOM	5241	CD2	LEU	262	6.679	-36.485	142.514	1.00	26.28	C	C
	ATOM	5242	C	LEU	262	5.749	-32.280	144.205	1.00	22.78	C	C
35	ATOM	5243	O	LEU	262	4.526	-32.149	144.249	1.00	21.96	C	O
	ATOM	5244	N	ALA	263	6.523	-32.150	145.279	1.00	21.56	C	N
	ATOM	5245	CA	ALA	263	5.960	-31.833	146.583	1.00	21.33	C	C
	ATOM	5246	CB	ALA	263	7.063	-31.825	147.648	1.00	19.74	C	C
	ATOM	5247	C	ALA	263	5.269	-30.469	146.531	1.00	20.96	C	C
40	ATOM	5248	O	ALA	263	4.220	-30.278	147.148	1.00	20.00	C	O
	ATOM	5249	N	ALA	264	5.865	-29.527	145.798	1.00	20.08	C	N
	ATOM	5250	CA	ALA	264	5.302	-28.187	145.663	1.00	21.05	C	C
	ATOM	5251	CB	ALA	264	6.243	-27.288	144.853	1.00	19.86	C	C
	ATOM	5252	C	ALA	264	3.943	-28.262	144.980	1.00	21.31	C	C
45	ATOM	5253	O	ALA	264	2.999	-27.590	145.394	1.00	21.71	C	O
	ATOM	5254	N	MET	265	3.852	-29.071	143.928	1.00	20.89	C	N
	ATOM	5255	CA	MET	265	2.597	-29.231	143.210	1.00	21.67	C	C
	ATOM	5256	CB	MET	265	2.804	-30.116	141.980	1.00	22.87	C	C
	ATOM	5257	CG	MET	265	3.497	-29.378	140.838	1.00	25.80	C	C
50	ATOM	5258	SD	MET	265	3.984	-30.411	139.427	1.00	29.35	C	S
	ATOM	5259	CE	MET	265	2.439	-30.483	138.513	1.00	26.54	C	C
	ATOM	5260	C	MET	265	1.515	-29.796	144.128	1.00	20.81	C	C
	ATOM	5261	O	MET	265	0.368	-29.372	144.066	1.00	19.86	C	O
	ATOM	5262	N	ALA	266	1.876	-30.739	144.992	1.00	20.98	C	N
55	ATOM	5263	CA	ALA	266	0.898	-31.300	145.922	1.00	21.57	C	C
	ATOM	5264	CB	ALA	266	1.494	-32.516	146.655	1.00	20.93	C	C
	ATOM	5265	C	ALA	266	0.473	-30.221	146.931	1.00	21.45	C	C
	ATOM	5266	O	ALA	266	-0.711	-30.083	147.254	1.00	20.27	C	O
	ATOM	5267	N	LEU	267	1.441	-29.455	147.425	1.00	21.93	C	N
	ATOM	5268	CA	LEU	267	1.156	-28.394	148.391	1.00	23.16	C	C
	ATOM	5269	CB	LEU	267	2.435	-27.635	148.751	1.00	23.06	C	C
	ATOM	5270	CG	LEU	267	2.553	-26.998	150.145	1.00	23.78	C	C

-260-

5	ATOM	5271	CD1	LEU	267	3.619	-25.911	150.100	1.00	23.35	C	C
	ATOM	5272	CD2	LEU	267	1.242	-26.417	150.605	1.00	23.37	C	C
	ATOM	5273	C	LEU	267	0.144	-27.390	147.838	1.00	23.66	C	C
	ATOM	5274	O	LEU	267	-0.862	-27.090	148.480	1.00	21.79	C	O
	ATOM	5275	N	PHE	268	0.421	-26.870	146.645	1.00	25.33	C	N
10	ATOM	5276	CA	PHE	268	-0.458	-25.881	146.031	1.00	27.92	C	C
	ATOM	5277	CB	PHE	268	0.358	-24.870	145.221	1.00	28.37	C	C
	ATOM	5278	CG	PHE	268	1.342	-24.097	146.048	1.00	28.12	C	C
	ATOM	5279	CD1	PHE	268	2.705	-24.256	145.856	1.00	27.58	C	C
	ATOM	5280	CD2	PHE	268	0.900	-23.252	147.061	1.00	28.65	C	C
15	ATOM	5281	CE1	PHE	268	3.620	-23.588	146.664	1.00	28.19	C	C
	ATOM	5282	CE2	PHE	268	1.805	-22.579	147.875	1.00	27.94	C	C
	ATOM	5283	CZ	PHE	268	3.167	-22.748	147.678	1.00	28.60	C	C
	ATOM	5284	C	PHE	268	-1.542	-26.480	145.155	1.00	29.29	C	C
	ATOM	5285	O	PHE	268	-1.512	-26.351	143.935	1.00	28.87	C	O
20	ATOM	5286	N	SER	269	-2.495	-27.141	145.800	1.00	31.35	C	N
	ATOM	5287	CA	SER	269	-3.625	-27.745	145.115	1.00	33.69	C	C
	ATOM	5288	CB	SER	269	-3.858	-29.168	145.616	1.00	33.87	C	C
	ATOM	5289	OG	SER	269	-2.838	-30.031	145.148	1.00	34.33	C	O
	ATOM	5290	C	SER	269	-4.822	-26.864	145.439	1.00	35.07	C	C
25	ATOM	5291	O	SER	269	-5.266	-26.801	146.587	1.00	34.90	C	O
	ATOM	5292	N	PRO	270	-5.350	-26.163	144.423	1.00	36.60	C	N
	ATOM	5293	CD	PRO	270	-4.922	-26.297	143.018	1.00	36.73	C	C
	ATOM	5294	CA	PRO	270	-6.495	-25.254	144.528	1.00	37.91	C	C
	ATOM	5295	CB	PRO	270	-6.556	-24.626	143.140	1.00	37.76	C	C
30	ATOM	5296	CG	PRO	270	-6.115	-25.758	142.262	1.00	37.41	C	C
	ATOM	5297	C	PRO	270	-7.806	-25.925	144.911	1.00	39.15	C	C
	ATOM	5298	O	PRO	270	-8.676	-25.296	145.514	1.00	39.22	C	O
	ATOM	5299	N	ASP	271	-7.942	-27.201	144.565	1.00	40.15	C	N
	ATOM	5300	CA	ASP	271	-9.158	-27.947	144.861	1.00	41.43	C	C
35	ATOM	5301	CB	ASP	271	-9.429	-28.966	143.749	1.00	42.35	C	C
	ATOM	5302	CG	ASP	271	-8.355	-30.041	143.658	1.00	43.65	C	C
	ATOM	5303	OD1	ASP	271	-7.150	-29.708	143.728	1.00	43.56	C	O
	ATOM	5304	OD2	ASP	271	-8.719	-31.227	143.499	1.00	44.16	C	O
	ATOM	5305	C	ASP	271	-9.090	-28.651	146.207	1.00	42.07	C	C
40	ATOM	5306	O	ASP	271	-9.604	-29.756	146.363	1.00	42.01	C	O
	ATOM	5307	N	ARG	272	-8.460	-27.999	147.178	1.00	42.23	C	N
	ATOM	5308	CA	ARG	272	-8.324	-28.552	148.516	1.00	42.88	C	C
	ATOM	5309	CB	ARG	272	-7.007	-28.084	149.139	1.00	42.11	C	C
	ATOM	5310	CG	ARG	272	-6.285	-29.134	149.948	1.00	41.65	C	C
45	ATOM	5311	CD	ARG	272	-5.106	-29.710	149.179	1.00	40.41	C	C
	ATOM	5312	NE	ARG	272	-5.240	-31.145	148.964	1.00	39.96	C	N
	ATOM	5313	CZ	ARG	272	-4.260	-31.951	148.563	1.00	38.64	C	C
	ATOM	5314	NH1	ARG	272	-3.045	-31.480	148.327	1.00	37.82	C	N
	ATOM	5315	NH2	ARG	272	-4.502	-33.240	148.387	1.00	37.11	C	N
50	ATOM	5316	C	ARG	272	-9.485	-28.073	149.385	1.00	44.03	C	C
	ATOM	5317	O	ARG	272	-9.942	-26.936	149.256	1.00	44.20	C	O
	ATOM	5318	N	PRO	273	-9.981	-28.933	150.284	1.00	44.99	C	N
	ATOM	5319	CD	PRO	273	-9.626	-30.345	150.507	1.00	45.02	C	C
	ATOM	5320	CA	PRO	273	-11.093	-28.528	151.150	1.00	45.66	C	C
55	ATOM	5321	CB	PRO	273	-11.443	-29.819	151.894	1.00	45.44	C	C
	ATOM	5322	CG	PRO	273	-10.156	-30.583	151.894	1.00	45.48	C	C
	ATOM	5323	C	PRO	273	-10.738	-27.379	152.096	1.00	46.37	C	C
	ATOM	5324	O	PRO	273	-9.806	-27.481	152.898	1.00	46.17	C	O
	ATOM	5325	N	GLY	274	-11.483	-26.282	151.986	1.00	47.11	C	N
	ATOM	5326	CA	GLY	274	-11.248	-25.130	152.839	1.00	47.72	C	C
	ATOM	5327	C	GLY	274	-10.538	-23.950	152.196	1.00	48.32	C	C
	ATOM	5328	O	GLY	274	-10.379	-22.908	152.830	1.00	48.57	C	O

-261-

	ATOM	5329	N	VAL	275	-10.113	-24.095	150.945	1.00	48.85	C	N
	ATOM	5330	CA	VAL	275	-9.411	-23.016	150.252	1.00	49.89	C	C
	ATOM	5331	CB	VAL	275	-8.810	-23.500	148.919	1.00	49.99	C	C
5	ATOM	5332	CG1	VAL	275	-7.739	-24.549	149.183	1.00	50.05	C	C
	ATOM	5333	CG2	VAL	275	-9.912	-24.060	148.025	1.00	50.42	C	C
	ATOM	5334	C	VAL	275	-10.289	-21.804	149.958	1.00	50.42	C	C
	ATOM	5335	O	VAL	275	-11.468	-21.939	149.631	1.00	49.97	C	O
	ATOM	5336	N	THR	276	-9.692	-20.620	150.072	1.00	51.16	C	N
10	ATOM	5337	CA	THR	276	-10.389	-19.365	149.813	1.00	51.63	C	C
	ATOM	5338	CB	THR	276	-10.118	-18.333	150.928	1.00	51.76	C	C
	ATOM	5339	OG1	THR	276	-10.588	-18.844	152.180	1.00	51.76	C	O
	ATOM	5340	CG2	THR	276	-10.830	-17.027	150.629	1.00	52.34	C	C
	ATOM	5341	C	THR	276	-9.924	-18.788	148.479	1.00	52.17	C	C
15	ATOM	5342	O	THR	276	-10.722	-18.611	147.558	1.00	52.52	C	O
	ATOM	5343	N	GLN	277	-8.629	-18.498	148.378	1.00	52.57	C	N
	ATOM	5344	CA	GLN	277	-8.053	-17.951	147.154	1.00	52.67	C	C
	ATOM	5345	CB	GLN	277	-6.759	-17.195	147.473	1.00	53.56	C	C
	ATOM	5346	CG	GLN	277	-6.913	-15.676	147.596	1.00	55.26	C	C
20	ATOM	5347	CD	GLN	277	-7.875	-15.252	148.694	1.00	56.34	C	C
	ATOM	5348	OE1	GLN	277	-9.070	-15.547	148.641	1.00	56.71	C	O
	ATOM	5349	NE2	GLN	277	-7.354	-14.551	149.698	1.00	56.69	C	N
	ATOM	5350	C	GLN	277	-7.773	-19.065	146.144	1.00	52.40	C	C
	ATOM	5351	O	GLN	277	-6.619	-19.374	145.847	1.00	51.95	C	O
25	ATOM	5352	N	ARG	278	-8.839	-19.654	145.609	1.00	52.21	C	N
	ATOM	5353	CA	ARG	278	-8.720	-20.740	144.644	1.00	52.47	C	C
	ATOM	5354	CB	ARG	278	-10.111	-21.228	144.226	1.00	54.03	C	C
	ATOM	5355	CG	ARG	278	-10.105	-22.600	143.568	1.00	56.61	C	C
	ATOM	5356	CD	ARG	278	-11.488	-23.005	143.074	1.00	58.62	C	C
30	ATOM	5357	NE	ARG	278	-11.550	-24.434	142.770	1.00	60.54	C	N
	ATOM	5358	CZ	ARG	278	-12.604	-25.056	142.245	1.00	61.18	C	C
	ATOM	5359	NH1	ARG	278	-13.712	-24.384	141.949	1.00	61.12	C	N
	ATOM	5360	NH2	ARG	278	-12.552	-26.364	142.022	1.00	61.81	C	N
	ATOM	5361	C	ARG	278	-7.922	-20.357	143.400	1.00	51.41	C	C
35	ATOM	5362	O	ARG	278	-7.084	-21.129	142.933	1.00	51.31	C	O
	ATOM	5363	N	ASP	279	-8.182	-19.170	142.861	1.00	50.43	C	N
	ATOM	5364	CA	ASP	279	-7.481	-18.710	141.668	1.00	48.92	C	C
	ATOM	5365	CB	ASP	279	-8.122	-17.431	141.123	1.00	50.20	C	C
	ATOM	5366	CG	ASP	279	-9.497	-17.675	140.530	1.00	51.42	C	C
40	ATOM	5367	OD1	ASP	279	-10.433	-17.982	141.296	1.00	52.30	C	O
	ATOM	5368	OD2	ASP	279	-9.640	-17.568	139.294	1.00	52.68	C	O
	ATOM	5369	C	ASP	279	-6.000	-18.469	141.916	1.00	47.51	C	C
	ATOM	5370	O	ASP	279	-5.163	-18.872	141.116	1.00	47.56	C	O
	ATOM	5371	N	GLU	280	-5.673	-17.806	143.019	1.00	46.03	C	N
45	ATOM	5372	CA	GLU	280	-4.276	-17.540	143.339	1.00	44.77	C	C
	ATOM	5373	CB	GLU	280	-4.178	-16.700	144.614	1.00	46.49	C	C
	ATOM	5374	CG	GLU	280	-2.776	-16.603	145.185	1.00	48.88	C	C
	ATOM	5375	CD	GLU	280	-2.682	-15.619	146.331	1.00	50.21	C	C
	ATOM	5376	OE1	GLU	280	-3.633	-15.555	147.141	1.00	51.50	C	O
50	ATOM	5377	OE2	GLU	280	-1.650	-14.920	146.430	1.00	51.27	C	O
	ATOM	5378	C	GLU	280	-3.488	-18.840	143.501	1.00	42.73	C	C
	ATOM	5379	O	GLU	280	-2.377	-18.965	142.994	1.00	42.02	C	O
	ATOM	5380	N	ILE	281	-4.069	-19.805	144.206	1.00	41.11	C	N
	ATOM	5381	CA	ILE	281	-3.415	-21.093	144.414	1.00	40.07	C	C
55	ATOM	5382	CB	ILE	281	-4.193	-21.952	145.439	1.00	38.98	C	C
	ATOM	5383	CG2	ILE	281	-3.628	-23.365	145.480	1.00	37.84	C	C
	ATOM	5384	CG1	ILE	281	-4.124	-21.291	146.820	1.00	38.21	C	C
	ATOM	5385	CD1	ILE	281	-4.957	-21.981	147.882	1.00	38.30	C	C
	ATOM	5386	C	ILE	281	-3.313	-21.835	143.081	1.00	40.18	C	C

-262-

	ATOM	5387	O	ILE	281	-2.318	-22.508	142.810	1.00	39.57	C	O
	ATOM	5388	N	ASP	282	-4.344	-21.692	142.252	1.00	40.74	C	N
	ATOM	5389	CA	ASP	282	-4.390	-22.319	140.934	1.00	41.64	C	C
5	ATOM	5390	CB	ASP	282	-5.695	-21.949	140.226	1.00	44.29	C	C
	ATOM	5391	CG	ASP	282	-6.024	-22.882	139.077	1.00	46.45	C	C
	ATOM	5392	OD1	ASP	282	-5.120	-23.187	138.270	1.00	48.25	C	O
	ATOM	5393	OD2	ASP	282	-7.196	-23.305	138.977	1.00	48.22	C	O
	ATOM	5394	C	ASP	282	-3.208	-21.835	140.099	1.00	41.04	C	C
10	ATOM	5395	O	ASP	282	-2.509	-22.629	139.470	1.00	40.33	C	O
	ATOM	5396	N	GLN	283	-2.997	-20.521	140.097	1.00	40.82	C	N
	ATOM	5397	CA	GLN	283	-1.899	-19.906	139.358	1.00	40.46	C	C
	ATOM	5398	CB	GLN	283	-1.966	-18.383	139.493	1.00	41.88	C	C
	ATOM	5399	CG	GLN	283	-0.695	-17.656	139.074	1.00	45.42	C	C
15	ATOM	5400	CD	GLN	283	-0.388	-17.788	137.591	1.00	47.59	C	C
	ATOM	5401	OE1	GLN	283	-0.244	-18.895	137.062	1.00	48.47	C	O
	ATOM	5402	NE2	GLN	283	-0.279	-16.652	136.913	1.00	49.11	C	N
	ATOM	5403	C	GLN	283	-0.557	-20.408	139.879	1.00	39.02	C	C
	ATOM	5404	O	GLN	283	0.381	-20.626	139.110	1.00	38.65	C	O
20	ATOM	5405	N	LEU	284	-0.470	-20.574	141.194	1.00	37.60	C	N
	ATOM	5406	CA	LEU	284	0.752	-21.060	141.824	1.00	36.30	C	C
	ATOM	5407	CB	LEU	284	0.595	-21.036	143.346	1.00	36.28	C	C
	ATOM	5408	CG	LEU	284	1.311	-19.955	144.172	1.00	36.05	C	C
	ATOM	5409	CD1	LEU	284	1.559	-18.694	143.366	1.00	35.74	C	C
25	ATOM	5410	CD2	LEU	284	0.474	-19.665	145.404	1.00	34.66	C	C
	ATOM	5411	C	LEU	284	1.068	-22.476	141.349	1.00	35.48	C	C
	ATOM	5412	O	LEU	284	2.217	-22.789	141.044	1.00	34.73	C	O
	ATOM	5413	N	GLN	285	0.054	-23.332	141.272	1.00	35.23	C	N
	ATOM	5414	CA	GLN	285	0.296	-24.698	140.828	1.00	35.83	C	C
30	ATOM	5415	CB	GLN	285	-0.968	-25.549	140.923	1.00	36.09	C	C
	ATOM	5416	CG	GLN	285	-0.661	-27.036	140.807	1.00	37.57	C	C
	ATOM	5417	CD	GLN	285	-1.863	-27.918	141.050	1.00	39.14	C	C
	ATOM	5418	OE1	GLN	285	-1.730	-29.033	141.555	1.00	40.08	C	O
	ATOM	5419	NE2	GLN	285	-3.047	-27.433	140.681	1.00	39.83	C	N
35	ATOM	5420	C	GLN	285	0.827	-24.727	139.401	1.00	35.60	C	C
	ATOM	5421	O	GLN	285	1.760	-25.473	139.096	1.00	35.31	C	O
	ATOM	5422	N	GLU	286	0.235	-23.920	138.526	1.00	35.27	C	N
	ATOM	5423	CA	GLU	286	0.688	-23.863	137.142	1.00	35.56	C	C
	ATOM	5424	CB	GLU	286	-0.192	-22.906	136.338	1.00	37.53	C	C
40	ATOM	5425	CG	GLU	286	-0.646	-23.468	134.997	1.00	41.47	C	C
	ATOM	5426	CD	GLU	286	0.216	-23.007	133.838	1.00	44.16	C	C
	ATOM	5427	OE1	GLU	286	0.381	-21.776	133.674	1.00	45.97	C	O
	ATOM	5428	OE2	GLU	286	0.715	-23.866	133.078	1.00	45.32	C	O
	ATOM	5429	C	GLU	286	2.154	-23.417	137.110	1.00	34.24	C	C
45	ATOM	5430	O	GLU	286	2.947	-23.927	136.325	1.00	33.97	C	O
	ATOM	5431	N	GLU	287	2.515	-22.467	137.968	1.00	33.47	C	N
	ATOM	5432	CA	GLU	287	3.901	-22.007	138.048	1.00	33.05	C	C
	ATOM	5433	CB	GLU	287	4.053	-20.934	139.131	1.00	34.71	C	C
	ATOM	5434	CG	GLU	287	3.671	-19.525	138.713	1.00	38.06	C	C
50	ATOM	5435	CD	GLU	287	3.826	-18.528	139.858	1.00	40.74	C	C
	ATOM	5436	OE1	GLU	287	4.883	-18.556	140.535	1.00	41.79	C	O
	ATOM	5437	OE2	GLU	287	2.899	-17.716	140.079	1.00	41.29	C	O
	ATOM	5438	C	GLU	287	4.807	-23.189	138.389	1.00	31.74	C	C
	ATOM	5439	O	GLU	287	5.877	-23.342	137.805	1.00	31.68	C	O
55	ATOM	5440	N	MET	288	4.380	-24.013	139.347	1.00	30.39	C	N
	ATOM	5441	CA	MET	288	5.155	-25.188	139.751	1.00	29.43	C	C
	ATOM	5442	CB	MET	288	4.491	-25.907	140.936	1.00	29.48	C	C
	ATOM	5443	CG	MET	288	4.242	-25.064	142.175	1.00	30.45	C	C
	ATOM	5444	SD	MET	288	5.726	-24.287	142.830	1.00	31.96	C	S

-263-

5	ATOM	5445	CE	MET	288	5.111	-22.620	143.124	1.00	33.18	C	C
	ATOM	5446	C	MET	288	5.250	-26.160	138.577	1.00	28.27	C	C
	ATOM	5447	O	MET	288	6.332	-26.608	138.212	1.00	27.19	C	O
	ATOM	5448	N	ALA	289	4.100	-26.478	137.992	1.00	28.27	C	N
	ATOM	5449	CA	ALA	289	4.025	-27.399	136.862	1.00	29.24	C	C
10	ATOM	5450	CB	ALA	289	2.585	-27.492	136.369	1.00	28.71	C	C
	ATOM	5451	C	ALA	289	4.944	-26.983	135.719	1.00	29.75	C	C
	ATOM	5452	O	ALA	289	5.729	-27.786	135.216	1.00	29.90	C	O
	ATOM	5453	N	LEU	290	4.838	-25.725	135.309	1.00	30.94	C	N
	ATOM	5454	CA	LEU	290	5.662	-25.196	134.233	1.00	32.24	C	C
15	ATOM	5455	CB	LEU	290	5.321	-23.723	134.000	1.00	33.16	C	C
	ATOM	5456	CG	LEU	290	4.598	-23.411	132.686	1.00	35.16	C	C
	ATOM	5457	CD1	LEU	290	3.515	-24.447	132.427	1.00	35.72	C	C
	ATOM	5458	CD2	LEU	290	4.002	-22.005	132.746	1.00	36.06	C	C
	ATOM	5459	C	LEU	290	7.137	-25.351	134.569	1.00	32.67	C	C
20	ATOM	5460	O	LEU	290	7.934	-25.771	133.734	1.00	32.95	C	O
	ATOM	5461	N	THR	291	7.501	-25.012	135.800	1.00	32.97	C	N
	ATOM	5462	CA	THR	291	8.884	-25.136	136.234	1.00	33.16	C	C
	ATOM	5463	CB	THR	291	9.051	-24.642	137.683	1.00	33.56	C	C
	ATOM	5464	OG1	THR	291	8.554	-23.303	137.783	1.00	32.87	C	O
25	ATOM	5465	CG2	THR	291	10.525	-24.666	138.092	1.00	32.59	C	C
	ATOM	5466	C	THR	291	9.331	-26.590	136.147	1.00	33.12	C	C
	ATOM	5467	O	THR	291	10.449	-26.878	135.722	1.00	32.77	C	O
	ATOM	5468	N	LEU	292	8.458	-27.509	136.556	1.00	33.66	C	N
	ATOM	5469	CA	LEU	292	8.781	-28.931	136.500	1.00	33.98	C	C
30	ATOM	5470	CB	LEU	292	7.641	-29.768	137.092	1.00	34.42	C	C
	ATOM	5471	CG	LEU	292	7.987	-31.152	137.659	1.00	34.71	C	C
	ATOM	5472	CD1	LEU	292	6.719	-31.972	137.772	1.00	34.26	C	C
	ATOM	5473	CD2	LEU	292	8.982	-31.871	136.782	1.00	34.52	C	C
	ATOM	5474	C	LEU	292	8.999	-29.339	135.042	1.00	34.02	C	C
35	ATOM	5475	O	LEU	292	9.975	-30.010	134.717	1.00	33.46	C	O
	ATOM	5476	N	GLN	293	8.076	-28.936	134.173	1.00	34.86	C	N
	ATOM	5477	CA	GLN	293	8.160	-29.261	132.752	1.00	36.35	C	C
	ATOM	5478	CB	GLN	293	6.971	-28.679	131.991	1.00	36.93	C	C
	ATOM	5479	CG	GLN	293	5.626	-29.178	132.436	1.00	38.19	C	C
40	ATOM	5480	CD	GLN	293	4.502	-28.583	131.612	1.00	39.76	C	C
	ATOM	5481	OE1	GLN	293	4.394	-28.839	130.409	1.00	39.18	C	O
	ATOM	5482	NE2	GLN	293	3.663	-27.772	132.254	1.00	39.83	C	N
	ATOM	5483	C	GLN	293	9.427	-28.683	132.161	1.00	37.04	C	C
	ATOM	5484	O	GLN	293	10.218	-29.389	131.540	1.00	36.18	C	O
45	ATOM	5485	N	SER	294	9.597	-27.379	132.353	1.00	38.14	C	N
	ATOM	5486	CA	SER	294	10.755	-26.661	131.856	1.00	39.42	C	C
	ATOM	5487	CB	SER	294	10.708	-25.213	132.343	1.00	39.88	C	C
	ATOM	5488	OG	SER	294	11.837	-24.490	131.897	1.00	42.89	C	O
	ATOM	5489	C	SER	294	12.030	-27.341	132.333	1.00	39.45	C	C
50	ATOM	5490	O	SER	294	12.966	-27.534	131.559	1.00	39.68	C	O
	ATOM	5491	N	TYR	295	12.061	-27.716	133.607	1.00	39.47	C	N
	ATOM	5492	CA	TYR	295	13.227	-28.382	134.160	1.00	39.54	C	C
	ATOM	5493	CB	TYR	295	13.083	-28.558	135.674	1.00	37.59	C	C
	ATOM	5494	CG	TYR	295	14.263	-29.263	136.310	1.00	35.04	C	C
55	ATOM	5495	CD1	TYR	295	14.398	-30.648	136.236	1.00	33.15	C	C
	ATOM	5496	CE1	TYR	295	15.498	-31.292	136.787	1.00	32.64	C	C
	ATOM	5497	CD2	TYR	295	15.264	-28.537	136.955	1.00	33.46	C	C
	ATOM	5498	CE2	TYR	295	16.370	-29.170	137.506	1.00	31.92	C	C
	ATOM	5499	CZ	TYR	295	16.481	-30.543	137.420	1.00	32.53	C	C
	ATOM	5500	OH	TYR	295	17.572	-31.169	137.968	1.00	33.06	C	O
	ATOM	5501	C	TYR	295	13.445	-29.736	133.501	1.00	40.70	C	C
	ATOM	5502	O	TYR	295	14.582	-30.137	133.283	1.00	41.09	C	O

-264-

	ATOM	5503	N	ILE	296	12.361	-30.445	133.200	1.00	42.17	C	N
	ATOM	5504	CA	ILE	296	12.467	-31.750	132.554	1.00	43.74	C	C
	ATOM	5505	CB	ILE	296	11.129	-32.538	132.634	1.00	42.58	C	C
5	ATOM	5506	CG2	ILE	296	11.179	-33.760	131.723	1.00	41.40	C	C
	ATOM	5507	CG1	ILE	296	10.864	-32.966	134.083	1.00	41.48	C	C
	ATOM	5508	CD1	ILE	296	9.588	-33.749	134.268	1.00	39.89	C	C
	ATOM	5509	C	ILE	296	12.887	-31.587	131.089	1.00	45.95	C	C
	ATOM	5510	O	ILE	296	13.719	-32.347	130.593	1.00	45.55	C	O
10	ATOM	5511	N	LYS	297	12.311	-30.605	130.399	1.00	48.91	C	N
	ATOM	5512	CA	LYS	297	12.675	-30.353	129.008	1.00	52.23	C	C
	ATOM	5513	CB	LYS	297	11.913	-29.150	128.441	1.00	51.99	C	C
	ATOM	5514	CG	LYS	297	10.439	-29.420	128.141	1.00	52.84	C	C
	ATOM	5515	CD	LYS	297	9.845	-28.308	127.281	1.00	53.70	C	C
15	ATOM	5516	CE	LYS	297	8.394	-28.574	126.904	1.00	54.12	C	C
	ATOM	5517	NZ	LYS	297	7.457	-28.404	128.051	1.00	54.87	C	N
	ATOM	5518	C	LYS	297	14.171	-30.082	129.014	1.00	54.53	C	C
	ATOM	5519	O	LYS	297	14.944	-30.844	128.441	1.00	55.09	C	O
20	ATOM	5520	N	GLY	298	14.584	-28.997	129.661	1.00	57.15	C	N
	ATOM	5521	CA	GLY	298	16.003	-28.724	129.748	1.00	60.22	C	C
	ATOM	5522	C	GLY	298	16.523	-29.978	130.411	1.00	62.54	C	C
	ATOM	5523	O	GLY	298	15.908	-30.455	131.358	1.00	62.69	C	O
	ATOM	5524	N	GLN	299	17.619	-30.541	129.922	1.00	65.17	C	N
	ATOM	5525	CA	GLN	299	18.124	-31.766	130.525	1.00	67.96	C	C
25	ATOM	5526	CB	GLN	299	18.292	-31.567	132.033	1.00	68.38	C	C
	ATOM	5527	CG	GLN	299	18.883	-32.742	132.776	1.00	69.15	C	C
	ATOM	5528	CD	GLN	299	18.708	-32.600	134.270	1.00	69.43	C	C
	ATOM	5529	OE1	GLN	299	17.601	-32.732	134.788	1.00	69.78	C	O
	ATOM	5530	NE2	GLN	299	19.798	-32.317	134.973	1.00	69.64	C	N
30	ATOM	5531	C	GLN	299	17.101	-32.871	130.246	1.00	69.68	C	C
	ATOM	5532	O	GLN	299	16.567	-33.497	131.167	1.00	69.64	C	O
	ATOM	5533	N	GLN	300	16.827	-33.082	128.961	1.00	71.61	C	N
	ATOM	5534	CA	GLN	300	15.871	-34.087	128.497	1.00	73.35	C	C
	ATOM	5535	CB	GLN	300	14.899	-33.450	127.502	1.00	73.72	C	C
35	ATOM	5536	CG	GLN	300	15.595	-32.770	126.322	1.00	74.58	C	C
	ATOM	5537	CD	GLN	300	14.762	-31.666	125.683	1.00	74.94	C	C
	ATOM	5538	OE1	GLN	300	15.233	-30.539	125.518	1.00	74.96	C	O
	ATOM	5539	NE2	GLN	300	13.525	-31.987	125.313	1.00	75.16	C	N
	ATOM	5540	C	GLN	300	16.613	-35.230	127.817	1.00	74.46	C	C
40	ATOM	5541	O	GLN	300	16.074	-35.910	126.943	1.00	74.52	C	O
	ATOM	5542	N	ARG	301	17.858	-35.433	128.228	1.00	75.88	C	N
	ATOM	5543	CA	ARG	301	18.695	-36.476	127.663	1.00	77.07	C	C
	ATOM	5544	CB	ARG	301	20.141	-36.271	128.128	1.00	77.84	C	C
	ATOM	5545	CG	ARG	301	20.867	-35.182	127.347	1.00	78.90	C	C
45	ATOM	5546	CD	ARG	301	22.091	-34.650	128.082	1.00	79.88	C	C
	ATOM	5547	NE	ARG	301	21.753	-33.615	129.060	1.00	80.47	C	N
	ATOM	5548	CZ	ARG	301	21.322	-32.392	128.754	1.00	80.79	C	C
	ATOM	5549	NH1	ARG	301	21.163	-32.022	127.488	1.00	80.67	C	N
	ATOM	5550	NH2	ARG	301	21.063	-31.525	129.723	1.00	81.13	C	N
50	ATOM	5551	C	ARG	301	18.209	-37.889	127.991	1.00	77.29	C	C
	ATOM	5552	O	ARG	301	17.149	-38.307	127.516	1.00	77.30	C	O
	ATOM	5553	N	ARG	302	18.978	-38.613	128.809	1.00	77.38	C	N
	ATOM	5554	CA	ARG	302	18.663	-39.998	129.179	1.00	77.29	C	C
	ATOM	5555	CB	ARG	302	17.389	-40.112	130.036	1.00	77.61	C	C
55	ATOM	5556	CG	ARG	302	16.778	-38.840	130.578	1.00	78.03	C	C
	ATOM	5557	CD	ARG	302	17.240	-38.614	131.998	1.00	78.58	C	C
	ATOM	5558	NE	ARG	302	18.590	-38.064	132.042	1.00	79.11	C	N
	ATOM	5559	CZ	ARG	302	18.889	-36.800	131.754	1.00	79.49	C	C
	ATOM	5560	NH1	ARG	302	17.931	-35.950	131.406	1.00	79.26	C	N

-265-

	ATOM	5561	NH2	ARG	302	20.148	-36.384	131.810	1.00	79.38	C	N
	ATOM	5562	C	ARG	302	18.380	-40.723	127.872	1.00	76.92	C	C
	ATOM	5563	O	ARG	302	18.585	-40.166	126.794	1.00	77.08	C	O
5	ATOM	5564	N	PRO	303	17.937	-41.991	127.942	1.00	76.31	C	N
	ATOM	5565	CD	PRO	303	18.164	-43.054	128.938	1.00	76.37	C	C
	ATOM	5566	CA	PRO	303	17.673	-42.587	126.631	1.00	75.50	C	C
	ATOM	5567	CB	PRO	303	17.382	-44.051	126.964	1.00	75.85	C	C
	ATOM	5568	CG	PRO	303	18.289	-44.303	128.053	1.00	76.19	C	C
10	ATOM	5569	C	PRO	303	16.497	-41.892	125.957	1.00	74.45	C	C
	ATOM	5570	O	PRO	303	16.409	-41.881	124.740	1.00	74.66	C	O
	ATOM	5571	N	ARG	304	15.590	-41.321	126.748	1.00	72.88	C	N
	ATOM	5572	CA	ARG	304	14.445	-40.604	126.185	1.00	71.00	C	C
	ATOM	5573	CB	ARG	304	13.553	-41.580	125.396	1.00	71.95	C	C
15	ATOM	5574	CG	ARG	304	13.004	-42.797	126.185	1.00	72.83	C	C
	ATOM	5575	CD	ARG	304	11.451	-42.760	126.214	1.00	73.75	C	C
	ATOM	5576	NE	ARG	304	10.894	-42.747	124.857	1.00	74.86	C	N
	ATOM	5577	CZ	ARG	304	10.661	-41.650	124.131	1.00	75.42	C	C
	ATOM	5578	NH1	ARG	304	10.905	-40.437	124.613	1.00	75.19	C	N
20	ATOM	5579	NH2	ARG	304	10.238	-41.763	122.880	1.00	75.41	C	N
	ATOM	5580	C	ARG	304	13.588	-39.801	127.189	1.00	68.99	C	C
	ATOM	5581	O	ARG	304	13.812	-38.612	127.391	1.00	69.10	C	O
	ATOM	5582	N	ASP	305	12.606	-40.478	127.783	1.00	66.12	C	N
	ATOM	5583	CA	ASP	305	11.654	-39.968	128.758	1.00	62.53	C	C
25	ATOM	5584	CB	ASP	305	12.303	-39.853	130.145	1.00	64.03	C	C
	ATOM	5585	CG	ASP	305	12.146	-41.126	130.972	1.00	65.08	C	C
	ATOM	5586	OD1	ASP	305	10.994	-41.568	131.169	1.00	65.82	C	O
	ATOM	5587	OD2	ASP	305	13.167	-41.689	131.418	1.00	65.99	C	O
	ATOM	5588	C	ASP	305	10.965	-38.666	128.422	1.00	59.48	C	C
30	ATOM	5589	O	ASP	305	11.262	-37.638	129.017	1.00	59.18	C	O
	ATOM	5590	N	ARG	306	10.064	-38.713	127.450	1.00	55.57	C	N
	ATOM	5591	CA	ARG	306	9.266	-37.556	127.069	1.00	51.44	C	C
	ATOM	5592	CB	ARG	306	9.127	-37.474	125.568	1.00	53.15	C	C
	ATOM	5593	CG	ARG	306	8.361	-38.617	125.009	1.00	55.42	C	C
35	ATOM	5594	CD	ARG	306	7.691	-38.219	123.755	1.00	57.72	C	C
	ATOM	5595	NE	ARG	306	8.629	-38.071	122.651	1.00	59.57	C	N
	ATOM	5596	CZ	ARG	306	8.600	-38.822	121.560	1.00	60.42	C	C
	ATOM	5597	NH1	ARG	306	7.690	-39.766	121.445	1.00	61.04	C	N
	ATOM	5598	NH2	ARG	306	9.463	-38.620	120.579	1.00	61.02	C	N
40	ATOM	5599	C	ARG	306	7.883	-37.863	127.671	1.00	47.25	C	C
	ATOM	5600	O	ARG	306	6.933	-37.092	127.544	1.00	45.71	C	O
	ATOM	5601	N	PHE	307	7.808	-39.018	128.327	1.00	42.87	C	N
	ATOM	5602	CA	PHE	307	6.626	-39.527	129.004	1.00	38.61	C	C
	ATOM	5603	CB	PHE	307	6.547	-41.038	128.787	1.00	38.35	C	C
	ATOM	5604	CG	PHE	307	6.278	-41.436	127.363	1.00	38.97	C	C
45	ATOM	5605	CD1	PHE	307	4.973	-41.477	126.876	1.00	38.81	C	C
	ATOM	5606	CD2	PHE	307	7.326	-41.746	126.497	1.00	38.13	C	C
	ATOM	5607	CE1	PHE	307	4.710	-41.820	125.544	1.00	38.93	C	C
	ATOM	5608	CE2	PHE	307	7.076	-42.089	125.165	1.00	38.71	C	C
50	ATOM	5609	CZ	PHE	307	5.762	-42.125	124.687	1.00	38.27	C	C
	ATOM	5610	C	PHE	307	6.775	-39.251	130.499	1.00	35.65	C	C
	ATOM	5611	O	PHE	307	5.870	-39.545	131.273	1.00	35.24	C	O
	ATOM	5612	N	LEU	308	7.916	-38.685	130.893	1.00	32.79	C	N
	ATOM	5613	CA	LEU	308	8.206	-38.415	132.299	1.00	30.05	C	C
	ATOM	5614	CB	LEU	308	9.637	-37.875	132.459	1.00	29.38	C	C
55	ATOM	5615	CG	LEU	308	10.442	-38.135	133.749	1.00	30.65	C	C
	ATOM	5616	CD1	LEU	308	11.014	-36.815	134.243	1.00	30.23	C	C
	ATOM	5617	CD2	LEU	308	9.601	-38.791	134.833	1.00	28.72	C	C
	ATOM	5618	C	LEU	308	7.224	-37.465	132.981	1.00	28.52	C	C

-266-

5	ATOM	5619	O	LEU	308	6.660	-37.796	134.026	1.00	26.62	C	O
	ATOM	5620	N	TYR	309	7.022	-36.285	132.404	1.00	26.74	C	N
	ATOM	5621	CA	TYR	309	6.110	-35.317	132.998	1.00	26.38	C	C
	ATOM	5622	CB	TYR	309	6.055	-34.046	132.147	1.00	26.27	C	C
	ATOM	5623	CG	TYR	309	5.169	-32.974	132.737	1.00	26.31	C	C
10	ATOM	5624	CD1	TYR	309	5.476	-32.390	133.966	1.00	25.78	C	C
	ATOM	5625	CE1	TYR	309	4.647	-31.424	134.531	1.00	26.17	C	C
	ATOM	5626	CD2	TYR	309	4.008	-32.561	132.082	1.00	26.61	C	C
	ATOM	5627	CE2	TYR	309	3.170	-31.593	132.639	1.00	26.55	C	C
	ATOM	5628	CZ	TYR	309	3.497	-31.033	133.862	1.00	26.04	C	C
15	ATOM	5629	OH	TYR	309	2.676	-30.088	134.423	1.00	26.95	C	O
	ATOM	5630	C	TYR	309	4.704	-35.901	133.145	1.00	25.65	C	C
	ATOM	5631	O	TYR	309	4.092	-35.805	134.206	1.00	24.69	C	O
	ATOM	5632	N	ALA	310	4.202	-36.507	132.073	1.00	25.00	C	N
	ATOM	5633	CA	ALA	310	2.878	-37.113	132.091	1.00	25.46	C	C
20	ATOM	5634	CB	ALA	310	2.562	-37.742	130.721	1.00	23.32	C	C
	ATOM	5635	C	ALA	310	2.789	-38.167	133.203	1.00	25.38	C	C
	ATOM	5636	O	ALA	310	1.793	-38.226	133.919	1.00	24.96	C	O
	ATOM	5637	N	LYS	311	3.823	-38.997	133.341	1.00	25.22	C	N
	ATOM	5638	CA	LYS	311	3.835	-40.019	134.386	1.00	25.29	C	C
25	ATOM	5639	CB	LYS	311	5.072	-40.909	134.264	1.00	27.18	C	C
	ATOM	5640	CG	LYS	311	5.041	-41.883	133.108	1.00	29.62	C	C
	ATOM	5641	CD	LYS	311	6.294	-42.744	133.111	1.00	32.10	C	C
	ATOM	5642	CE	LYS	311	6.291	-43.739	131.963	1.00	33.43	C	C
	ATOM	5643	NZ	LYS	311	7.545	-44.543	131.967	1.00	36.49	C	N
30	ATOM	5644	C	LYS	311	3.817	-39.386	135.785	1.00	24.36	C	C
	ATOM	5645	O	LYS	311	3.206	-39.927	136.709	1.00	23.40	C	O
	ATOM	5646	N	LEU	312	4.491	-38.250	135.938	1.00	22.72	C	N
	ATOM	5647	CA	LEU	312	4.525	-37.566	137.227	1.00	22.36	C	C
	ATOM	5648	CB	LEU	312	5.615	-36.487	137.243	1.00	20.77	C	C
35	ATOM	5649	CG	LEU	312	7.066	-36.994	137.252	1.00	20.74	C	C
	ATOM	5650	CD1	LEU	312	8.025	-35.805	137.282	1.00	19.34	C	C
	ATOM	5651	CD2	LEU	312	7.300	-37.895	138.474	1.00	20.28	C	C
	ATOM	5652	C	LEU	312	3.160	-36.961	137.568	1.00	22.23	C	C
	ATOM	5653	O	LEU	312	2.787	-36.889	138.739	1.00	22.33	C	O
40	ATOM	5654	N	LEU	313	2.415	-36.517	136.562	1.00	21.95	C	N
	ATOM	5655	CA	LEU	313	1.087	-35.978	136.835	1.00	22.37	C	C
	ATOM	5656	CB	LEU	313	0.499	-35.292	135.597	1.00	21.79	C	C
	ATOM	5657	CG	LEU	313	1.160	-33.976	135.184	1.00	22.17	C	C
	ATOM	5658	CD1	LEU	313	0.375	-33.363	134.037	1.00	22.22	C	C
45	ATOM	5659	CD2	LEU	313	1.200	-33.010	136.371	1.00	21.19	C	C
	ATOM	5660	C	LEU	313	0.200	-37.146	137.266	1.00	22.14	C	C
	ATOM	5661	O	LEU	313	-0.610	-37.019	138.180	1.00	22.77	C	O
	ATOM	5662	N	GLY	314	0.368	-38.288	136.609	1.00	21.90	C	N
	ATOM	5663	CA	GLY	314	-0.409	-39.458	136.965	1.00	22.13	C	C
50	ATOM	5664	C	GLY	314	-0.117	-39.885	138.393	1.00	22.23	C	C
	ATOM	5665	O	GLY	314	-1.022	-40.283	139.124	1.00	21.32	C	O
	ATOM	5666	N	LEU	315	1.153	-39.809	138.790	1.00	22.49	C	N
	ATOM	5667	CA	LEU	315	1.550	-40.183	140.140	1.00	22.84	C	C
	ATOM	5668	CB	LEU	315	3.077	-40.249	140.250	1.00	23.35	C	C
55	ATOM	5669	CG	LEU	315	3.674	-41.496	139.587	1.00	23.08	C	C
	ATOM	5670	CD1	LEU	315	5.189	-41.400	139.500	1.00	22.58	C	C
	ATOM	5671	CD2	LEU	315	3.254	-42.716	140.396	1.00	22.20	C	C
	ATOM	5672	C	LEU	315	0.978	-39.208	141.158	1.00	23.01	C	C
	ATOM	5673	O	LEU	315	0.611	-39.610	142.262	1.00	23.00	C	O
	ATOM	5674	N	LEU	316	0.904	-37.929	140.793	1.00	22.90	C	N
	ATOM	5675	CA	LEU	316	0.329	-36.931	141.686	1.00	23.06	C	C
	ATOM	5676	CB	LEU	316	0.493	-35.518	141.116	1.00	22.05	C	C

-267-

5	ATOM	5677	CG	LEU	316	1.871	-34.892	141.360	1.00	23.73	C	C
	ATOM	5678	CD1	LEU	316	1.971	-33.540	140.669	1.00	23.24	C	C
	ATOM	5679	CD2	LEU	316	2.097	-34.745	142.861	1.00	23.94	C	C
	ATOM	5680	C	LEU	316	-1.148	-37.250	141.884	1.00	23.27	C	C
	ATOM	5681	O	LEU	316	-1.690	-37.080	142.981	1.00	22.65	C	O
10	ATOM	5682	N	ALA	317	-1.797	-37.715	140.817	1.00	23.25	C	N
	ATOM	5683	CA	ALA	317	-3.206	-38.089	140.888	1.00	24.23	C	C
	ATOM	5684	CB	ALA	317	-3.747	-38.378	139.489	1.00	22.85	C	C
	ATOM	5685	C	ALA	317	-3.335	-39.331	141.775	1.00	24.41	C	C
	ATOM	5686	O	ALA	317	-4.238	-39.424	142.606	1.00	24.43	C	O
15	ATOM	5687	N	GLU	318	-2.421	-40.279	141.603	1.00	24.78	C	N
	ATOM	5688	CA	GLU	318	-2.438	-41.500	142.398	1.00	26.34	C	C
	ATOM	5689	CB	GLU	318	-1.353	-42.469	141.918	1.00	28.61	C	C
	ATOM	5690	CG	GLU	318	-1.413	-43.829	142.596	1.00	33.39	C	C
	ATOM	5691	CD	GLU	318	-0.543	-44.866	141.906	1.00	36.18	C	C
20	ATOM	5692	OE1	GLU	318	-0.627	-44.984	140.665	1.00	38.18	C	O
	ATOM	5693	OE2	GLU	318	0.215	-45.571	142.603	1.00	38.68	C	O
	ATOM	5694	C	GLU	318	-2.227	-41.194	143.877	1.00	24.85	C	C
	ATOM	5695	O	GLU	318	-2.849	-41.810	144.740	1.00	23.99	C	O
	ATOM	5696	N	LEU	319	-1.347	-40.241	144.165	1.00	23.52	C	N
25	ATOM	5697	CA	LEU	319	-1.066	-39.850	145.541	1.00	23.29	C	C
	ATOM	5698	CB	LEU	319	0.106	-38.866	145.564	1.00	22.68	C	C
	ATOM	5699	CG	LEU	319	0.728	-38.525	146.917	1.00	23.73	C	C
	ATOM	5700	CD1	LEU	319	1.006	-39.791	147.707	1.00	21.67	C	C
	ATOM	5701	CD2	LEU	319	2.011	-37.730	146.683	1.00	23.23	C	C
30	ATOM	5702	C	LEU	319	-2.330	-39.226	146.144	1.00	22.92	C	C
	ATOM	5703	O	LEU	319	-2.593	-39.340	147.340	1.00	20.62	C	O
	ATOM	5704	N	ARG	320	-3.114	-38.569	145.297	1.00	23.19	C	N
	ATOM	5705	CA	ARG	320	-4.364	-37.967	145.727	1.00	24.36	C	C
	ATOM	5706	CB	ARG	320	-4.968	-37.168	144.577	1.00	26.94	C	C
35	ATOM	5707	CG	ARG	320	-6.167	-36.349	144.952	1.00	30.73	C	C
	ATOM	5708	CD	ARG	320	-5.770	-34.977	145.472	1.00	33.34	C	C
	ATOM	5709	NE	ARG	320	-6.959	-34.240	145.887	1.00	35.45	C	N
	ATOM	5710	CZ	ARG	320	-7.089	-32.919	145.846	1.00	36.12	C	C
	ATOM	5711	NH1	ARG	320	-6.096	-32.157	145.403	1.00	36.02	C	N
40	ATOM	5712	NH2	ARG	320	-8.222	-32.363	146.254	1.00	36.33	C	N
	ATOM	5713	C	ARG	320	-5.316	-39.099	146.148	1.00	23.68	C	C
	ATOM	5714	O	ARG	320	-6.003	-38.996	147.162	1.00	22.64	C	O
	ATOM	5715	N	SER	321	-5.350	-40.177	145.366	1.00	22.83	C	N
	ATOM	5716	CA	SER	321	-6.194	-41.336	145.675	1.00	22.71	C	C
45	ATOM	5717	CB	SER	321	-6.100	-42.394	144.571	1.00	22.94	C	C
	ATOM	5718	OG	SER	321	-6.657	-41.916	143.365	1.00	26.35	C	O
	ATOM	5719	C	SER	321	-5.757	-41.973	146.985	1.00	21.50	C	C
	ATOM	5720	O	SER	321	-6.585	-42.420	147.766	1.00	21.06	C	O
	ATOM	5721	N	ILE	322	-4.448	-42.031	147.208	1.00	20.81	C	N
50	ATOM	5722	CA	ILE	322	-3.905	-42.605	148.428	1.00	20.53	C	C
	ATOM	5723	CB	ILE	322	-2.357	-42.707	148.336	1.00	20.88	C	C
	ATOM	5724	CG2	ILE	322	-1.741	-42.841	149.730	1.00	20.05	C	C
	ATOM	5725	CG1	ILE	322	-1.980	-43.902	147.444	1.00	20.98	C	C
	ATOM	5726	CD1	ILE	322	-0.504	-43.985	147.088	1.00	20.14	C	C
55	ATOM	5727	C	ILE	322	-4.327	-41.754	149.629	1.00	20.03	C	C
	ATOM	5728	O	ILE	322	-4.642	-42.281	150.693	1.00	18.41	C	O
	ATOM	5729	N	ASN	323	-4.328	-40.437	149.442	1.00	20.64	C	N
	ATOM	5730	CA	ASN	323	-4.735	-39.483	150.478	1.00	22.57	C	C
	ATOM	5731	CB	ASN	323	-4.665	-38.049	149.925	1.00	24.66	C	C
55	ATOM	5732	CG	ASN	323	-5.148	-36.998	150.922	1.00	27.77	C	C
	ATOM	5733	OD1	ASN	323	-6.252	-37.087	151.463	1.00	28.78	C	O
	ATOM	5734	ND2	ASN	323	-4.323	-35.986	151.151	1.00	29.48	C	N

-268-

5	ATOM	5735	C	ASN	323	-6.172	-39.813	150.869	1.00	22.69	C	C
	ATOM	5736	O	ASN	323	-6.497	-39.936	152.053	1.00	22.78	C	O
	ATOM	5737	N	GLU	324	-7.025	-39.959	149.859	1.00	22.11	C	N
	ATOM	5738	CA	GLU	324	-8.427	-40.294	150.070	1.00	23.38	C	C
	ATOM	5739	CB	GLU	324	-9.186	-40.263	148.740	1.00	24.94	C	C
10	ATOM	5740	CG	GLU	324	-9.451	-38.866	148.200	1.00	28.85	C	C
	ATOM	5741	CD	GLU	324	-10.021	-38.887	146.791	1.00	31.28	C	C
	ATOM	5742	OE1	GLU	324	-10.867	-39.760	146.498	1.00	34.04	C	O
	ATOM	5743	OE2	GLU	324	-9.629	-38.028	145.976	1.00	32.20	C	O
	ATOM	5744	C	GLU	324	-8.591	-41.673	150.714	1.00	22.12	C	C
15	ATOM	5745	O	GLU	324	-9.446	-41.856	151.575	1.00	21.79	C	O
	ATOM	5746	N	ALA	325	-7.781	-42.641	150.297	1.00	20.25	C	N
	ATOM	5747	CA	ALA	325	-7.880	-43.982	150.869	1.00	20.09	C	C
	ATOM	5748	CB	ALA	325	-6.978	-44.958	150.112	1.00	20.27	C	C
	ATOM	5749	C	ALA	325	-7.527	-43.946	152.354	1.00	19.28	C	C
20	ATOM	5750	O	ALA	325	-8.133	-44.654	153.155	1.00	20.38	C	O
	ATOM	5751	N	TYR	326	-6.554	-43.121	152.728	1.00	18.75	C	N
	ATOM	5752	CA	TYR	326	-6.189	-42.974	154.140	1.00	19.01	C	C
	ATOM	5753	CB	TYR	326	-5.147	-41.869	154.325	1.00	18.00	C	C
	ATOM	5754	CG	TYR	326	-3.719	-42.355	154.417	1.00	18.20	C	C
25	ATOM	5755	CD1	TYR	326	-3.279	-43.109	155.513	1.00	17.45	C	C
	ATOM	5756	CE1	TYR	326	-1.943	-43.507	155.625	1.00	15.87	C	C
	ATOM	5757	CD2	TYR	326	-2.793	-42.022	153.433	1.00	17.03	C	C
	ATOM	5758	CE2	TYR	326	-1.466	-42.411	153.536	1.00	16.49	C	C
	ATOM	5759	CZ	TYR	326	-1.045	-43.148	154.633	1.00	16.11	C	C
30	ATOM	5760	OH	TYR	326	0.281	-43.497	154.719	1.00	14.54	C	O
	ATOM	5761	C	TYR	326	-7.437	-42.601	154.936	1.00	19.02	C	C
	ATOM	5762	O	TYR	326	-7.673	-43.127	156.029	1.00	16.95	C	O
	ATOM	5763	N	GLY	327	-8.223	-41.676	154.382	1.00	18.76	C	N
	ATOM	5764	CA	GLY	327	-9.448	-41.253	155.036	1.00	20.32	C	C
35	ATOM	5765	C	GLY	327	-10.379	-42.434	155.263	1.00	21.04	C	C
	ATOM	5766	O	GLY	327	-10.973	-42.576	156.329	1.00	20.76	C	O
	ATOM	5767	N	TYR	328	-10.516	-43.289	154.257	1.00	21.82	C	N
	ATOM	5768	CA	TYR	328	-11.366	-44.463	154.398	1.00	22.78	C	C
	ATOM	5769	CB	TYR	328	-11.461	-45.200	153.055	1.00	24.82	C	C
40	ATOM	5770	CG	TYR	328	-12.248	-46.491	153.120	1.00	27.89	C	C
	ATOM	5771	CD1	TYR	328	-11.645	-47.675	153.544	1.00	28.22	C	C
	ATOM	5772	CE1	TYR	328	-12.380	-48.852	153.680	1.00	29.71	C	C
	ATOM	5773	CD2	TYR	328	-13.615	-46.516	152.823	1.00	29.15	C	C
	ATOM	5774	CE2	TYR	328	-14.362	-47.693	152.959	1.00	30.37	C	C
45	ATOM	5775	CZ	TYR	328	-13.734	-48.853	153.391	1.00	29.77	C	C
	ATOM	5776	OH	TYR	328	-14.458	-50.005	153.567	1.00	31.94	C	O
	ATOM	5777	C	TYR	328	-10.792	-45.376	155.495	1.00	22.29	C	C
	ATOM	5778	O	TYR	328	-11.513	-45.818	156.391	1.00	21.48	C	O
	ATOM	5779	N	GLN	329	-9.493	-45.648	155.427	1.00	22.12	C	N
50	ATOM	5780	CA	GLN	329	-8.833	-46.490	156.424	1.00	22.84	C	C
	ATOM	5781	CB	GLN	329	-7.314	-46.491	156.205	1.00	21.43	C	C
	ATOM	5782	CG	GLN	329	-6.863	-47.132	154.901	1.00	20.52	C	C
	ATOM	5783	CD	GLN	329	-7.302	-48.581	154.789	1.00	21.36	C	C
	ATOM	5784	OE1	GLN	329	-8.063	-48.948	153.889	1.00	21.96	C	O
55	ATOM	5785	NE2	GLN	329	-6.831	-49.413	155.712	1.00	17.88	C	N
	ATOM	5786	C	GLN	329	-9.131	-46.003	157.846	1.00	24.04	C	C
	ATOM	5787	O	GLN	329	-9.506	-46.794	158.719	1.00	24.21	C	O
	ATOM	5788	N	ILE	330	-8.963	-44.703	158.070	1.00	24.50	C	N
	ATOM	5789	CA	ILE	330	-9.186	-44.099	159.382	1.00	26.20	C	C
55	ATOM	5790	CB	ILE	330	-8.698	-42.611	159.395	1.00	27.02	C	C
	ATOM	5791	CG2	ILE	330	-9.413	-41.804	160.470	1.00	26.57	C	C
	ATOM	5792	CG1	ILE	330	-7.196	-42.562	159.670	1.00	28.06	C	C

-269-

	ATOM	5793	CD1	ILE	330	-6.343	-43.192	158.615	1.00	29.01	C	C
	ATOM	5794	C	ILE	330	-10.634	-44.175	159.876	1.00	26.85	C	C
	ATOM	5795	O	ILE	330	-10.879	-44.240	161.079	1.00	24.12	C	O
5	ATOM	5796	N	GLN	331	-11.594	-44.164	158.959	1.00	28.57	C	N
	ATOM	5797	CA	GLN	331	-12.987	-44.244	159.373	1.00	31.36	C	C
	ATOM	5798	CB	GLN	331	-13.887	-43.474	158.389	1.00	34.12	C	C
	ATOM	5799	CG	GLN	331	-14.097	-44.139	157.027	1.00	40.12	C	C
	ATOM	5800	CD	GLN	331	-15.111	-45.281	157.055	1.00	43.64	C	C
10	ATOM	5801	OE1	GLN	331	-14.886	-46.346	156.463	1.00	46.08	C	O
	ATOM	5802	NE2	GLN	331	-16.234	-45.062	157.737	1.00	45.76	C	N
	ATOM	5803	C	GLN	331	-13.455	-45.700	159.493	1.00	30.71	C	C
	ATOM	5804	O	GLN	331	-14.393	-45.995	160.220	1.00	30.97	C	O
	ATOM	5805	N	HIS	332	-12.778	-46.608	158.801	1.00	30.40	C	N
15	ATOM	5806	CA	HIS	332	-13.154	-48.017	158.802	1.00	29.57	C	C
	ATOM	5807	CB	HIS	332	-12.897	-48.605	157.411	1.00	30.43	C	C
	ATOM	5808	CG	HIS	332	-13.480	-49.969	157.209	1.00	32.56	C	C
	ATOM	5809	CD2	HIS	332	-12.898	-51.148	156.881	1.00	33.11	C	C
	ATOM	5810	ND1	HIS	332	-14.830	-50.225	157.314	1.00	33.92	C	N
20	ATOM	5811	CE1	HIS	332	-15.055	-51.502	157.057	1.00	33.97	C	C
	ATOM	5812	NE2	HIS	332	-13.899	-52.084	156.791	1.00	33.45	C	N
	ATOM	5813	C	HIS	332	-12.471	-48.881	159.861	1.00	28.67	C	C
	ATOM	5814	O	HIS	332	-13.054	-49.855	160.333	1.00	28.01	C	O
	ATOM	5815	N	ILE	333	-11.248	-48.532	160.247	1.00	27.55	C	N
25	ATOM	5816	CA	ILE	333	-10.541	-49.336	161.237	1.00	26.64	C	C
	ATOM	5817	CB	ILE	333	-9.264	-49.938	160.623	1.00	26.21	C	C
	ATOM	5818	CG2	ILE	333	-8.508	-50.761	161.662	1.00	26.49	C	C
	ATOM	5819	CG1	ILE	333	-9.653	-50.844	159.447	1.00	25.58	C	C
	ATOM	5820	CD1	ILE	333	-8.831	-50.630	158.209	1.00	24.86	C	C
30	ATOM	5821	C	ILE	333	-10.211	-48.587	162.519	1.00	26.30	C	C
	ATOM	5822	O	ILE	333	-9.405	-47.660	162.525	1.00	26.27	C	O
	ATOM	5823	N	GLN	334	-10.853	-49.009	163.605	1.00	25.96	C	N
	ATOM	5824	CA	GLN	334	-10.678	-48.412	164.929	1.00	26.54	C	C
	ATOM	5825	CB	GLN	334	-11.595	-49.132	165.923	1.00	28.84	C	C
35	ATOM	5826	CG	GLN	334	-11.621	-48.572	167.336	1.00	32.45	C	C
	ATOM	5827	CD	GLN	334	-12.537	-49.386	168.254	1.00	36.09	C	C
	ATOM	5828	OE1	GLN	334	-12.079	-50.041	169.198	1.00	37.52	C	O
	ATOM	5829	NE2	GLN	334	-13.840	-49.355	167.969	1.00	37.02	C	N
	ATOM	5830	C	GLN	334	-9.222	-48.497	165.394	1.00	25.97	C	C
40	ATOM	5831	O	GLN	334	-8.584	-49.547	165.271	1.00	25.42	C	O
	ATOM	5832	N	GLY	335	-8.699	-47.390	165.919	1.00	25.33	C	N
	ATOM	5833	CA	GLY	335	-7.324	-47.365	166.392	1.00	24.56	C	C
	ATOM	5834	C	GLY	335	-6.324	-46.695	165.465	1.00	24.72	C	C
	ATOM	5835	O	GLY	335	-5.318	-46.141	165.917	1.00	24.71	C	O
45	ATOM	5836	N	LEU	336	-6.586	-46.744	164.166	1.00	24.12	C	N
	ATOM	5837	CA	LEU	336	-5.695	-46.131	163.194	1.00	24.24	C	C
	ATOM	5838	CB	LEU	336	-6.186	-46.398	161.771	1.00	23.67	C	C
	ATOM	5839	CG	LEU	336	-6.009	-47.818	161.229	1.00	25.15	C	C
	ATOM	5840	CD1	LEU	336	-6.539	-47.886	159.795	1.00	24.62	C	C
50	ATOM	5841	CD2	LEU	336	-4.530	-48.207	161.277	1.00	24.69	C	C
	ATOM	5842	C	LEU	336	-5.541	-44.626	163.390	1.00	23.69	C	C
	ATOM	5843	O	LEU	336	-4.432	-44.102	163.348	1.00	23.11	C	O
	ATOM	5844	N	SER	337	-6.653	-43.930	163.598	1.00	23.42	C	N
	ATOM	5845	CA	SER	337	-6.610	-42.481	163.771	1.00	23.59	C	C
55	ATOM	5846	CB	SER	337	-8.012	-41.931	164.044	1.00	23.77	C	C
	ATOM	5847	OG	SER	337	-8.473	-42.375	165.303	1.00	27.27	C	O
	ATOM	5848	C	SER	337	-5.671	-42.044	164.889	1.00	22.01	C	C
	ATOM	5849	O	SER	337	-5.089	-40.967	164.824	1.00	22.40	C	O
	ATOM	5850	N	ALA	338	-5.517	-42.882	165.907	1.00	21.30	C	N

-270-

5	ATOM	5851	CA	ALA	338	-4.649	-42.568	167.038	1.00	21.23	C	C
	ATOM	5852	CB	ALA	338	-4.786	-43.660	168.118	1.00	19.99	C	C
	ATOM	5853	C	ALA	338	-3.170	-42.372	166.665	1.00	20.93	C	C
	ATOM	5854	O	ALA	338	-2.408	-41.788	167.440	1.00	20.73	C	O
	ATOM	5855	N	MET	339	-2.763	-42.862	165.494	1.00	21.18	C	N
10	ATOM	5856	CA	MET	339	-1.380	-42.709	165.037	1.00	21.93	C	C
	ATOM	5857	CB	MET	339	-0.995	-43.866	164.117	1.00	20.73	C	C
	ATOM	5858	CG	MET	339	-0.835	-45.183	164.865	1.00	19.60	C	C
	ATOM	5859	SD	MET	339	-0.305	-46.523	163.803	1.00	19.45	C	S
	ATOM	5860	CE	MET	339	-1.798	-46.789	162.824	1.00	19.70	C	C
15	ATOM	5861	C	MET	339	-1.146	-41.369	164.335	1.00	22.95	C	C
	ATOM	5862	O	MET	339	-0.029	-41.034	163.945	1.00	21.85	C	O
	ATOM	5863	N	MET	340	-2.219	-40.614	164.167	1.00	24.72	C	N
	ATOM	5864	CA	MET	340	-2.154	-39.292	163.568	1.00	27.94	C	C
	ATOM	5865	CB	MET	340	-2.843	-39.296	162.207	1.00	27.04	C	C
20	ATOM	5866	CG	MET	340	-2.692	-38.005	161.453	1.00	26.07	C	C
	ATOM	5867	SD	MET	340	-0.965	-37.738	161.038	1.00	25.64	C	S
	ATOM	5868	CE	MET	340	-1.132	-36.639	159.656	1.00	24.53	C	C
	ATOM	5869	C	MET	340	-2.965	-38.472	164.558	1.00	31.10	C	C
	ATOM	5870	O	MET	340	-3.995	-37.911	164.193	1.00	29.95	C	O
25	ATOM	5871	N	PRO	341	-2.499	-38.393	165.825	1.00	34.82	C	N
	ATOM	5872	CD	PRO	341	-1.062	-38.551	166.110	1.00	34.96	C	C
	ATOM	5873	CA	PRO	341	-3.138	-37.674	166.934	1.00	38.26	C	C
	ATOM	5874	CB	PRO	341	-1.981	-37.433	167.904	1.00	37.12	C	C
	ATOM	5875	CG	PRO	341	-0.800	-37.386	167.016	1.00	35.89	C	C
30	ATOM	5876	C	PRO	341	-3.801	-36.398	166.490	1.00	41.84	C	C
	ATOM	5877	O	PRO	341	-4.568	-36.386	165.531	1.00	43.72	C	O
	ATOM	5878	N	LEU	342	-3.555	-35.309	167.196	1.00	44.96	C	N
	ATOM	5879	CA	LEU	342	-4.134	-34.079	166.723	1.00	46.88	C	C
	ATOM	5880	CB	LEU	342	-3.876	-32.930	167.708	1.00	48.46	C	C
35	ATOM	5881	CG	LEU	342	-4.775	-32.923	168.952	1.00	49.28	C	C
	ATOM	5882	CD1	LEU	342	-4.242	-33.902	169.995	1.00	50.51	C	C
	ATOM	5883	CD2	LEU	342	-4.833	-31.520	169.532	1.00	50.29	C	C
	ATOM	5884	C	LEU	342	-3.331	-33.917	165.437	1.00	47.75	C	C
	ATOM	5885	O	LEU	342	-2.870	-34.907	164.857	1.00	46.19	C	O
40	ATOM	5886	N	LEU	343	-3.141	-32.691	164.982	1.00	48.81	C	N
	ATOM	5887	CA	LEU	343	-2.374	-32.508	163.767	1.00	49.66	C	C
	ATOM	5888	CB	LEU	343	-1.024	-33.243	163.875	1.00	47.94	C	C
	ATOM	5889	CG	LEU	343	0.102	-32.825	164.841	1.00	46.64	C	C
	ATOM	5890	CD1	LEU	343	0.840	-31.632	164.275	1.00	46.63	C	C
45	ATOM	5891	CD2	LEU	343	-0.438	-32.523	166.230	1.00	46.74	C	C
	ATOM	5892	C	LEU	343	-3.196	-33.071	162.607	1.00	51.07	C	C
	ATOM	5893	O	LEU	343	-3.014	-34.222	162.192	1.00	50.79	C	O
	ATOM	5894	N	GLN	344	-4.133	-32.254	162.125	1.00	53.04	C	N
	ATOM	5895	CA	GLN	344	-4.988	-32.595	160.988	1.00	55.20	C	C
50	ATOM	5896	CB	GLN	344	-4.103	-32.912	159.782	1.00	55.64	C	C
	ATOM	5897	CG	GLN	344	-2.891	-31.999	159.666	1.00	56.26	C	C
	ATOM	5898	CD	GLN	344	-1.728	-32.654	158.953	1.00	57.17	C	C
	ATOM	5899	OE1	GLN	344	-0.631	-32.105	158.912	1.00	57.87	C	O
	ATOM	5900	NE2	GLN	344	-1.960	-33.830	158.384	1.00	57.99	C	N
55	ATOM	5901	C	GLN	344	-5.979	-33.743	161.207	1.00	56.43	C	C
	ATOM	5902	O	GLN	344	-6.823	-34.001	160.349	1.00	56.91	C	O
	ATOM	5903	N	GLU	345	-5.872	-34.430	162.343	1.00	57.98	C	N
	ATOM	5904	CA	GLU	345	-6.749	-35.555	162.680	1.00	58.92	C	C
	ATOM	5905	CB	GLU	345	-8.215	-35.106	162.696	1.00	59.25	C	C
	ATOM	5906	CG	GLU	345	-8.449	-33.790	163.412	1.00	60.42	C	C
	ATOM	5907	CD	GLU	345	-8.699	-32.648	162.449	1.00	60.91	C	C
	ATOM	5908	OE1	GLU	345	-8.396	-31.491	162.807	1.00	61.74	C	O

-271-

5	ATOM	5909	OE2	GLU	345	-9.205	-32.905	161.336	1.00	61.02	C	O
	ATOM	5910	C	GLU	345	-6.591	-36.739	161.719	1.00	59.19	C	C
	ATOM	5911	O	GLU	345	-5.784	-36.638	160.768	1.00	59.25	C	O
	ATOM	5912	OXT	GLU	345	-7.281	-37.761	161.931	1.00	59.81	C	O
	TER	5913		GLU	345						C	
10	ATOM	5914	CB	PRO	103	-18.301	-92.854	125.997	1.00	85.60	D	C
	ATOM	5915	CG	PRO	103	-19.706	-93.039	125.435	1.00	85.87	D	C
	ATOM	5916	C	PRO	103	-16.716	-90.915	125.789	1.00	84.96	D	C
	ATOM	5917	O	PRO	103	-16.171	-90.150	126.588	1.00	85.09	D	O
	ATOM	5918	N	PRO	103	-19.062	-90.839	124.910	1.00	85.59	D	N
15	ATOM	5919	CD	PRO	103	-19.833	-91.960	124.343	1.00	85.67	D	C
	ATOM	5920	CA	PRO	103	-18.173	-91.336	125.986	1.00	85.36	D	C
	ATOM	5921	N	VAL	104	-16.100	-91.423	124.722	1.00	84.12	D	N
	ATOM	5922	CA	VAL	104	-14.705	-91.134	124.383	1.00	83.16	D	C
	ATOM	5923	CB	VAL	104	-14.383	-89.620	124.512	1.00	83.15	D	C
20	ATOM	5924	CG1	VAL	104	-12.923	-89.364	124.170	1.00	83.06	D	C
	ATOM	5925	CG2	VAL	104	-15.285	-88.818	123.588	1.00	83.15	D	C
	ATOM	5926	C	VAL	104	-13.719	-91.938	125.235	1.00	82.38	D	C
	ATOM	5927	O	VAL	104	-13.000	-92.790	124.709	1.00	82.56	D	O
	ATOM	5928	N	GLN	105	-13.680	-91.678	126.541	1.00	81.19	D	N
25	ATOM	5929	CA	GLN	105	-12.769	-92.406	127.423	1.00	79.59	D	C
	ATOM	5930	CB	GLN	105	-11.313	-92.048	127.082	1.00	80.41	D	C
	ATOM	5931	CG	GLN	105	-10.285	-93.137	127.413	1.00	81.01	D	C
	ATOM	5932	CD	GLN	105	-10.121	-93.381	128.905	1.00	81.38	D	C
	ATOM	5933	OE1	GLN	105	-9.699	-92.494	129.648	1.00	81.47	D	O
30	ATOM	5934	NE2	GLN	105	-10.452	-94.591	129.348	1.00	81.27	D	N
	ATOM	5935	C	GLN	105	-13.029	-92.153	128.912	1.00	77.80	D	C
	ATOM	5936	O	GLN	105	-12.190	-91.579	129.607	1.00	77.77	D	O
	ATOM	5937	N	LEU	106	-14.196	-92.573	129.394	1.00	75.34	D	N
	ATOM	5938	CA	LEU	106	-14.548	-92.421	130.806	1.00	72.86	D	C
35	ATOM	5939	CB	LEU	106	-15.641	-91.358	131.007	1.00	72.85	D	C
	ATOM	5940	CG	LEU	106	-17.068	-91.595	130.507	1.00	72.73	D	C
	ATOM	5941	CD1	LEU	106	-17.971	-90.477	131.006	1.00	72.42	D	C
	ATOM	5942	CD2	LEU	106	-17.083	-91.663	128.995	1.00	72.91	D	C
	ATOM	5943	C	LEU	106	-15.024	-93.774	131.322	1.00	70.93	D	C
40	ATOM	5944	O	LEU	106	-16.207	-93.981	131.588	1.00	70.45	D	O
	ATOM	5945	N	SER	107	-14.074	-94.693	131.450	1.00	68.94	D	N
	ATOM	5946	CA	SER	107	-14.343	-96.045	131.910	1.00	67.00	D	C
	ATOM	5947	CB	SER	107	-13.023	-96.776	132.172	1.00	66.72	D	C
	ATOM	5948	OG	SER	107	-12.247	-96.102	133.146	1.00	65.92	D	O
45	ATOM	5949	C	SER	107	-15.208	-96.096	133.160	1.00	65.96	D	C
	ATOM	5950	O	SER	107	-15.463	-95.079	133.806	1.00	65.94	D	O
	ATOM	5951	N	LYS	108	-15.666	-97.297	133.489	1.00	64.35	D	N
	ATOM	5952	CA	LYS	108	-16.489	-97.493	134.669	1.00	62.78	D	C
	ATOM	5953	CB	LYS	108	-17.282	-98.798	134.547	1.00	63.38	D	C
50	ATOM	5954	CG	LYS	108	-18.220	-98.836	133.341	1.00	64.14	D	C
	ATOM	5955	CD	LYS	108	-19.192	-97.657	133.350	1.00	65.05	D	C
	ATOM	5956	CE	LYS	108	-20.081	-97.638	132.112	1.00	65.31	D	C
	ATOM	5957	NZ	LYS	108	-19.304	-97.432	130.858	1.00	65.55	D	N
	ATOM	5958	C	LYS	108	-15.607	-97.516	135.917	1.00	61.20	D	C
55	ATOM	5959	O	LYS	108	-16.086	-97.290	137.025	1.00	60.95	D	O
	ATOM	5960	N	GLU	109	-14.317	-97.787	135.731	1.00	59.39	D	N
	ATOM	5961	CA	GLU	109	-13.374	-97.822	136.840	1.00	57.92	D	C
	ATOM	5962	CB	GLU	109	-12.017	-98.381	136.392	1.00	58.83	D	C
	ATOM	5963	CG	GLU	109	-12.031	-99.817	135.870	1.00	60.46	D	C
	ATOM	5964	CD	GLU	109	-12.296	-99.909	134.372	1.00	61.30	D	C
	ATOM	5965	OE1	GLU	109	-13.443	-99.660	133.936	1.00	61.45	D	O
	ATOM	5966	OE2	GLU	109	-11.344	-100.228	133.626	1.00	61.74	D	O

-272-

	ATOM	5967	C	GLU	109	-13.182	-96.405	137.372	1.00	56.28	D	C
	ATOM	5968	O	GLU	109	-13.311	-96.156	138.571	1.00	56.26	D	O
	ATOM	5969	N	GLN	110	-12.872	-95.476	136.473	1.00	53.97	D	N
5	ATOM	5970	CA	GLN	110	-12.669	-94.090	136.868	1.00	51.62	D	C
	ATOM	5971	CB	GLN	110	-11.900	-93.336	135.775	1.00	51.23	D	C
	ATOM	5972	CG	GLN	110	-12.575	-93.289	134.422	1.00	50.22	D	C
	ATOM	5973	CD	GLN	110	-11.624	-92.904	133.295	1.00	49.90	D	C
	ATOM	5974	OE1	GLN	110	-12.062	-92.493	132.223	1.00	49.66	D	O
10	ATOM	5975	NE2	GLN	110	-10.320	-93.051	133.528	1.00	49.10	D	N
	ATOM	5976	C	GLN	110	-14.002	-93.410	137.190	1.00	50.17	D	C
	ATOM	5977	O	GLN	110	-14.042	-92.403	137.893	1.00	49.22	D	O
	ATOM	5978	N	GLU	111	-15.098	-93.965	136.683	1.00	48.81	D	N
	ATOM	5979	CA	GLU	111	-16.415	-93.418	136.984	1.00	47.31	D	C
15	ATOM	5980	CB	GLU	111	-17.461	-93.987	136.020	1.00	49.14	D	C
	ATOM	5981	CG	GLU	111	-18.809	-93.276	136.069	1.00	51.36	D	C
	ATOM	5982	CD	GLU	111	-19.723	-93.664	134.914	1.00	53.11	D	C
	ATOM	5983	OE1	GLU	111	-20.068	-94.862	134.793	1.00	53.51	D	O
	ATOM	5984	OE2	GLU	111	-20.098	-92.765	134.126	1.00	53.59	D	O
20	ATOM	5985	C	GLU	111	-16.748	-93.798	138.440	1.00	45.08	D	C
	ATOM	5986	O	GLU	111	-17.479	-93.089	139.127	1.00	44.43	D	O
	ATOM	5987	N	GLU	112	-16.191	-94.919	138.896	1.00	42.54	D	N
	ATOM	5988	CA	GLU	112	-16.378	-95.401	140.263	1.00	40.31	D	C
	ATOM	5989	CB	GLU	112	-16.100	-96.912	140.331	1.00	40.53	D	C
25	ATOM	5990	CG	GLU	112	-15.884	-97.484	141.744	1.00	41.61	D	C
	ATOM	5991	CD	GLU	112	-17.127	-97.436	142.629	1.00	41.94	D	C
	ATOM	5992	OE1	GLU	112	-17.006	-97.761	143.831	1.00	42.13	D	O
	ATOM	5993	OE2	GLU	112	-18.219	-97.081	142.129	1.00	41.78	D	O
	ATOM	5994	C	GLU	112	-15.425	-94.644	141.199	1.00	38.58	D	C
30	ATOM	5995	O	GLU	112	-15.752	-94.396	142.358	1.00	37.73	D	O
	ATOM	5996	N	LEU	113	-14.245	-94.289	140.690	1.00	36.41	D	N
	ATOM	5997	CA	LEU	113	-13.262	-93.541	141.469	1.00	34.41	D	C
	ATOM	5998	CB	LEU	113	-11.978	-93.348	140.660	1.00	34.39	D	C
	ATOM	5999	CG	LEU	113	-10.991	-92.312	141.214	1.00	34.64	D	C
35	ATOM	6000	CD1	LEU	113	-10.423	-92.785	142.556	1.00	33.12	D	C
	ATOM	6001	CD2	LEU	113	-9.879	-92.084	140.200	1.00	34.83	D	C
	ATOM	6002	C	LEU	113	-13.837	-92.169	141.840	1.00	33.24	D	C
	ATOM	6003	O	LEU	113	-13.663	-91.692	142.961	1.00	32.72	D	O
	ATOM	6004	N	ILE	114	-14.503	-91.534	140.881	1.00	31.70	D	N
40	ATOM	6005	CA	ILE	114	-15.114	-90.233	141.109	1.00	31.14	D	C
	ATOM	6006	CB	ILE	114	-15.682	-89.644	139.794	1.00	30.51	D	C
	ATOM	6007	CG2	ILE	114	-16.572	-88.445	140.087	1.00	28.60	D	C
	ATOM	6008	CG1	ILE	114	-14.528	-89.234	138.870	1.00	30.78	D	C
	ATOM	6009	CD1	ILE	114	-14.985	-88.681	137.532	1.00	29.75	D	C
45	ATOM	6010	C	ILE	114	-16.237	-90.357	142.140	1.00	31.12	D	C
	ATOM	6011	O	ILE	114	-16.382	-89.501	143.015	1.00	30.80	D	O
	ATOM	6012	N	ARG	115	-17.025	-91.426	142.035	1.00	30.77	D	N
	ATOM	6013	CA	ARG	115	-18.127	-91.657	142.968	1.00	30.08	D	C
	ATOM	6014	CB	ARG	115	-18.843	-92.972	142.640	1.00	31.12	D	C
50	ATOM	6015	CG	ARG	115	-20.155	-93.160	143.393	1.00	32.38	D	C
	ATOM	6016	CD	ARG	115	-20.721	-94.563	143.216	1.00	33.88	D	C
	ATOM	6017	NE	ARG	115	-19.921	-95.576	143.907	1.00	34.78	D	N
	ATOM	6018	CZ	ARG	115	-19.824	-95.701	145.232	1.00	35.85	D	C
	ATOM	6019	NH1	ARG	115	-20.479	-94.880	146.048	1.00	35.62	D	N
55	ATOM	6020	NH2	ARG	115	-19.056	-96.653	145.746	1.00	35.96	D	N
	ATOM	6021	C	ARG	115	-17.587	-91.726	144.393	1.00	28.71	D	C
	ATOM	6022	O	ARG	115	-18.126	-91.102	145.301	1.00	28.14	D	O
	ATOM	6023	N	THR	116	-16.514	-92.491	144.559	1.00	27.78	D	N
	ATOM	6024	CA	THR	116	-15.850	-92.705	145.837	1.00	27.53	D	C

-273-

5	ATOM	6025	CB	THR	116	-14.748	-93.769	145.676	1.00	28.08	D	C
	ATOM	6026	OG1	THR	116	-15.353	-95.009	145.288	1.00	30.70	D	O
	ATOM	6027	CG2	THR	116	-13.978	-93.964	146.978	1.00	29.30	D	C
	ATOM	6028	C	THR	116	-15.233	-91.439	146.435	1.00	26.60	D	C
	ATOM	6029	O	THR	116	-15.435	-91.134	147.616	1.00	25.28	D	O
10	ATOM	6030	N	LEU	117	-14.467	-90.715	145.622	1.00	24.99	D	N
	ATOM	6031	CA	LEU	117	-13.831	-89.486	146.080	1.00	23.90	D	C
	ATOM	6032	CB	LEU	117	-12.951	-88.902	144.969	1.00	22.02	D	C
	ATOM	6033	CG	LEU	117	-11.621	-89.624	144.740	1.00	20.36	D	C
	ATOM	6034	CD1	LEU	117	-10.988	-89.149	143.448	1.00	19.86	D	C
15	ATOM	6035	CD2	LEU	117	-10.698	-89.379	145.920	1.00	19.89	D	C
	ATOM	6036	C	LEU	117	-14.882	-88.469	146.493	1.00	23.81	D	C
	ATOM	6037	O	LEU	117	-14.759	-87.823	147.533	1.00	23.44	D	O
	ATOM	6038	N	LEU	118	-15.920	-88.345	145.668	1.00	23.97	D	N
	ATOM	6039	CA	LEU	118	-17.008	-87.409	145.908	1.00	24.68	D	C
20	ATOM	6040	CB	LEU	118	-17.918	-87.350	144.680	1.00	26.07	D	C
	ATOM	6041	CG	LEU	118	-18.967	-86.236	144.665	1.00	27.99	D	C
	ATOM	6042	CD1	LEU	118	-18.298	-84.877	144.878	1.00	28.05	D	C
	ATOM	6043	CD2	LEU	118	-19.703	-86.266	143.329	1.00	29.41	D	C
	ATOM	6044	C	LEU	118	-17.825	-87.775	147.144	1.00	24.04	D	C
25	ATOM	6045	O	LEU	118	-18.187	-86.907	147.936	1.00	23.27	D	O
	ATOM	6046	N	GLY	119	-18.128	-89.061	147.295	1.00	23.56	D	N
	ATOM	6047	CA	GLY	119	-18.886	-89.501	148.451	1.00	22.61	D	C
	ATOM	6048	C	GLY	119	-18.142	-89.112	149.714	1.00	22.12	D	C
	ATOM	6049	O	GLY	119	-18.715	-88.489	150.610	1.00	21.52	D	O
30	ATOM	6050	N	ALA	120	-16.860	-89.471	149.776	1.00	21.08	D	N
	ATOM	6051	CA	ALA	120	-16.025	-89.163	150.931	1.00	21.42	D	C
	ATOM	6052	CB	ALA	120	-14.643	-89.795	150.761	1.00	20.72	D	C
	ATOM	6053	C	ALA	120	-15.886	-87.657	151.131	1.00	21.67	D	C
	ATOM	6054	O	ALA	120	-15.933	-87.158	152.251	1.00	21.20	D	O
35	ATOM	6055	N	HIS	121	-15.713	-86.933	150.037	1.00	21.91	D	N
	ATOM	6056	CA	HIS	121	-15.563	-85.493	150.118	1.00	22.79	D	C
	ATOM	6057	CB	HIS	121	-15.227	-84.923	148.734	1.00	23.76	D	C
	ATOM	6058	CG	HIS	121	-15.230	-83.429	148.680	1.00	24.65	D	C
	ATOM	6059	CD2	HIS	121	-14.268	-82.525	148.980	1.00	25.00	D	C
40	ATOM	6060	ND1	HIS	121	-16.337	-82.700	148.300	1.00	25.79	D	N
	ATOM	6061	CE1	HIS	121	-16.057	-81.410	148.366	1.00	25.43	D	C
	ATOM	6062	NE2	HIS	121	-14.807	-81.277	148.777	1.00	26.28	D	N
	ATOM	6063	C	HIS	121	-16.823	-84.834	150.674	1.00	22.33	D	C
	ATOM	6064	O	HIS	121	-16.748	-83.978	151.557	1.00	21.50	D	O
45	ATOM	6065	N	THR	122	-17.977	-85.234	150.156	1.00	21.62	D	N
	ATOM	6066	CA	THR	122	-19.249	-84.673	150.597	1.00	22.81	D	C
	ATOM	6067	CB	THR	122	-20.414	-85.242	149.772	1.00	23.18	D	C
	ATOM	6068	OG1	THR	122	-20.194	-84.954	148.387	1.00	25.50	D	O
	ATOM	6069	CG2	THR	122	-21.729	-84.624	150.212	1.00	22.28	D	C
50	ATOM	6070	C	THR	122	-19.528	-84.934	152.077	1.00	22.45	D	C
	ATOM	6071	O	THR	122	-19.981	-84.043	152.796	1.00	21.90	D	O
	ATOM	6072	N	ARG	123	-19.257	-86.153	152.527	1.00	21.68	D	N
	ATOM	6073	CA	ARG	123	-19.487	-86.502	153.922	1.00	22.61	D	C
	ATOM	6074	CB	ARG	123	-19.269	-88.008	154.149	1.00	22.11	D	C
55	ATOM	6075	CG	ARG	123	-20.308	-88.924	153.500	1.00	24.00	D	C
	ATOM	6076	CD	ARG	123	-20.170	-90.366	153.975	1.00	23.54	D	C
	ATOM	6077	NE	ARG	123	-18.996	-91.050	153.438	1.00	24.44	D	N
	ATOM	6078	CZ	ARG	123	-18.905	-91.554	152.207	1.00	25.95	D	C
	ATOM	6079	NH1	ARG	123	-19.919	-91.461	151.356	1.00	24.95	D	N
	ATOM	6080	NH2	ARG	123	-17.794	-92.170	151.828	1.00	26.27	D	N
	ATOM	6081	C	ARG	123	-18.606	-85.742	154.914	1.00	22.53	D	C
	ATOM	6082	O	ARG	123	-19.091	-85.245	155.929	1.00	22.70	D	O

-274-

5	ATOM	6083	N	HIS	124	-17.318	-85.634	154.604	1.00	22.37	D	N
	ATOM	6084	CA	HIS	124	-16.359	-85.028	155.524	1.00	22.99	D	C
	ATOM	6085	CB	HIS	124	-15.223	-86.027	155.732	1.00	23.32	D	C
	ATOM	6086	CG	HIS	124	-15.699	-87.397	156.093	1.00	25.33	D	C
	ATOM	6087	CD2	HIS	124	-16.458	-87.831	157.128	1.00	24.81	D	C
10	ATOM	6088	ND1	HIS	124	-15.444	-88.505	155.313	1.00	25.61	D	N
	ATOM	6089	CE1	HIS	124	-16.028	-89.561	155.851	1.00	25.40	D	C
	ATOM	6090	NE2	HIS	124	-16.650	-89.179	156.953	1.00	24.90	D	N
	ATOM	6091	C	HIS	124	-15.751	-83.643	155.284	1.00	22.18	D	C
	ATOM	6092	O	HIS	124	-15.365	-82.975	156.243	1.00	22.39	D	O
15	ATOM	6093	N	MET	125	-15.652	-83.202	154.038	1.00	21.09	D	N
	ATOM	6094	CA	MET	125	-15.040	-81.902	153.790	1.00	21.77	D	C
	ATOM	6095	CB	MET	125	-13.752	-82.093	152.992	1.00	21.06	D	C
	ATOM	6096	CG	MET	125	-12.741	-82.995	153.689	1.00	21.90	D	C
	ATOM	6097	SD	MET	125	-11.145	-83.007	152.872	1.00	24.77	D	S
20	ATOM	6098	CE	MET	125	-11.623	-83.594	151.192	1.00	24.05	D	C
	ATOM	6099	C	MET	125	-15.898	-80.833	153.128	1.00	21.17	D	C
	ATOM	6100	O	MET	125	-15.870	-79.681	153.549	1.00	21.24	D	O
	ATOM	6101	N	GLY	126	-16.654	-81.220	152.104	1.00	21.62	D	N
	ATOM	6102	CA	GLY	126	-17.499	-80.296	151.364	1.00	22.06	D	C
25	ATOM	6103	C	GLY	126	-18.159	-79.155	152.113	1.00	23.28	D	C
	ATOM	6104	O	GLY	126	-18.209	-78.027	151.619	1.00	23.14	D	O
	ATOM	6105	N	THR	127	-18.694	-79.433	153.296	1.00	23.58	D	N
	ATOM	6106	CA	THR	127	-19.340	-78.387	154.071	1.00	24.53	D	C
	ATOM	6107	CB	THR	127	-20.870	-78.636	154.170	1.00	25.29	D	C
30	ATOM	6108	OG1	THR	127	-21.119	-80.020	154.456	1.00	25.66	D	O
	ATOM	6109	CG2	THR	127	-21.560	-78.260	152.856	1.00	25.86	D	C
	ATOM	6110	C	THR	127	-18.754	-78.256	155.473	1.00	24.35	D	C
	ATOM	6111	O	THR	127	-19.414	-77.759	156.387	1.00	24.95	D	O
	ATOM	6112	N	MET	128	-17.509	-78.686	155.651	1.00	23.31	D	N
35	ATOM	6113	CA	MET	128	-16.898	-78.600	156.969	1.00	22.39	D	C
	ATOM	6114	CB	MET	128	-15.534	-79.308	156.981	1.00	21.54	D	C
	ATOM	6115	CG	MET	128	-14.357	-78.513	156.440	1.00	19.76	D	C
	ATOM	6116	SD	MET	128	-12.852	-79.535	156.386	1.00	18.11	D	S
	ATOM	6117	CE	MET	128	-11.875	-78.626	155.196	1.00	18.78	D	C
40	ATOM	6118	C	MET	128	-16.764	-77.146	157.437	1.00	21.87	D	C
	ATOM	6119	O	MET	128	-16.694	-76.889	158.635	1.00	20.88	D	O
	ATOM	6120	N	PHE	129	-16.759	-76.202	156.496	1.00	20.44	D	N
	ATOM	6121	CA	PHE	129	-16.649	-74.779	156.822	1.00	22.40	D	C
	ATOM	6122	CB	PHE	129	-16.515	-73.947	155.521	1.00	23.38	D	C
45	ATOM	6123	CG	PHE	129	-17.793	-73.839	154.716	1.00	24.91	D	C
	ATOM	6124	CD1	PHE	129	-18.787	-72.934	155.076	1.00	26.36	D	C
	ATOM	6125	CD2	PHE	129	-18.005	-74.651	153.608	1.00	26.00	D	C
	ATOM	6126	CE1	PHE	129	-19.976	-72.840	154.344	1.00	27.45	D	C
	ATOM	6127	CE2	PHE	129	-19.187	-74.568	152.869	1.00	26.23	D	C
50	ATOM	6128	CZ	PHE	129	-20.174	-73.661	153.239	1.00	26.91	D	C
	ATOM	6129	C	PHE	129	-17.823	-74.260	157.682	1.00	22.06	D	C
	ATOM	6130	O	PHE	129	-17.687	-73.264	158.394	1.00	20.89	D	O
	ATOM	6131	N	GLU	130	-18.969	-74.936	157.625	1.00	23.03	D	N
	ATOM	6132	CA	GLU	130	-20.135	-74.530	158.416	1.00	24.67	D	C
55	ATOM	6133	CB	GLU	130	-21.389	-75.306	157.978	1.00	26.82	D	C
	ATOM	6134	CG	GLU	130	-21.913	-74.974	156.573	1.00	29.47	D	C
	ATOM	6135	CD	GLU	130	-22.531	-73.581	156.467	1.00	32.46	D	C
	ATOM	6136	OE1	GLU	130	-22.560	-72.847	157.480	1.00	34.27	D	O
	ATOM	6137	OE2	GLU	130	-22.994	-73.216	155.362	1.00	33.81	D	O
	ATOM	6138	C	GLU	130	-19.905	-74.751	159.916	1.00	23.97	D	C
	ATOM	6139	O	GLU	130	-20.622	-74.199	160.745	1.00	24.44	D	O
	ATOM	6140	N	GLN	131	-18.907	-75.563	160.257	1.00	22.76	D	N

-275-

	ATOM	6141	CA	GLN	131	-18.589	-75.853	161.652	1.00	22.20	D	C
	ATOM	6142	CB	GLN	131	-17.967	-77.245	161.778	1.00	24.32	D	C
	ATOM	6143	CG	GLN	131	-18.846	-78.385	161.290	1.00	28.51	D	C
5	ATOM	6144	CD	GLN	131	-20.204	-78.392	161.961	1.00	31.63	D	C
	ATOM	6145	OE1	GLN	131	-20.305	-78.373	163.193	1.00	34.51	D	O
	ATOM	6146	NE2	GLN	131	-21.259	-78.420	161.154	1.00	32.89	D	N
	ATOM	6147	C	GLN	131	-17.627	-74.843	162.269	1.00	20.71	D	C
	ATOM	6148	O	GLN	131	-17.440	-74.829	163.483	1.00	19.33	D	O
10	ATOM	6149	N	PHE	132	-17.010	-74.007	161.439	1.00	18.82	D	N
	ATOM	6150	CA	PHE	132	-16.055	-73.025	161.939	1.00	18.21	D	C
	ATOM	6151	CB	PHE	132	-15.547	-72.129	160.798	1.00	17.25	D	C
	ATOM	6152	CG	PHE	132	-14.612	-72.825	159.823	1.00	16.76	D	C
	ATOM	6153	CD1	PHE	132	-14.178	-74.133	160.039	1.00	15.85	D	C
	ATOM	6154	CD2	PHE	132	-14.151	-72.150	158.694	1.00	15.94	D	C
15	ATOM	6155	CE1	PHE	132	-13.299	-74.762	159.141	1.00	16.23	D	C
	ATOM	6156	CE2	PHE	132	-13.268	-72.772	157.789	1.00	16.64	D	C
	ATOM	6157	CZ	PHE	132	-12.843	-74.078	158.017	1.00	15.57	D	C
	ATOM	6158	C	PHE	132	-16.641	-72.159	163.050	1.00	17.13	D	C
20	ATOM	6159	O	PHE	132	-15.946	-71.802	163.993	1.00	16.35	D	O
	ATOM	6160	N	VAL	133	-17.921	-71.832	162.942	1.00	16.80	D	N
	ATOM	6161	CA	VAL	133	-18.584	-71.011	163.949	1.00	18.67	D	C
	ATOM	6162	CB	VAL	133	-20.010	-70.597	163.480	1.00	18.65	D	C
	ATOM	6163	CG1	VAL	133	-20.978	-71.762	163.626	1.00	18.17	D	C
	ATOM	6164	CG2	VAL	133	-20.484	-69.400	164.272	1.00	21.43	D	C
25	ATOM	6165	C	VAL	133	-18.675	-71.698	165.327	1.00	18.01	D	C
	ATOM	6166	O	VAL	133	-19.034	-71.058	166.314	1.00	17.64	D	O
	ATOM	6167	N	GLN	134	-18.348	-72.989	165.383	1.00	17.24	D	N
	ATOM	6168	CA	GLN	134	-18.360	-73.760	166.631	1.00	18.01	D	C
	ATOM	6169	CB	GLN	134	-18.574	-75.250	166.332	1.00	18.24	D	C
30	ATOM	6170	CG	GLN	134	-19.887	-75.587	165.643	1.00	20.23	D	C
	ATOM	6171	CD	GLN	134	-21.072	-75.499	166.579	1.00	20.77	D	C
	ATOM	6172	OE1	GLN	134	-21.701	-76.506	166.899	1.00	22.88	D	O
	ATOM	6173	NE2	GLN	134	-21.377	-74.298	167.032	1.00	20.71	D	N
	ATOM	6174	C	GLN	134	-17.038	-73.616	167.390	1.00	18.05	D	C
35	ATOM	6175	O	GLN	134	-16.900	-74.102	168.514	1.00	17.44	D	O
	ATOM	6176	N	PHE	135	-16.067	-72.944	166.778	1.00	17.41	D	N
	ATOM	6177	CA	PHE	135	-14.754	-72.808	167.392	1.00	17.91	D	C
	ATOM	6178	CB	PHE	135	-13.699	-73.329	166.412	1.00	16.42	D	C
	ATOM	6179	CG	PHE	135	-13.864	-74.794	166.091	1.00	15.86	D	C
40	ATOM	6180	CD1	PHE	135	-13.423	-75.766	166.982	1.00	16.41	D	C
	ATOM	6181	CD2	PHE	135	-14.525	-75.198	164.942	1.00	15.95	D	C
	ATOM	6182	CE1	PHE	135	-13.641	-77.127	166.737	1.00	17.52	D	C
	ATOM	6183	CE2	PHE	135	-14.756	-76.563	164.678	1.00	16.49	D	C
	ATOM	6184	CZ	PHE	135	-14.311	-77.526	165.581	1.00	16.50	D	C
45	ATOM	6185	C	PHE	135	-14.399	-71.421	167.909	1.00	18.76	D	C
	ATOM	6186	O	PHE	135	-13.288	-70.915	167.703	1.00	19.28	D	O
	ATOM	6187	N	ARG	136	-15.360	-70.813	168.590	1.00	19.27	D	N
	ATOM	6188	CA	ARG	136	-15.167	-69.511	169.198	1.00	20.81	D	C
	ATOM	6189	CB	ARG	136	-14.265	-69.678	170.428	1.00	22.56	D	C
50	ATOM	6190	CG	ARG	136	-14.890	-70.539	171.538	1.00	26.27	D	C
	ATOM	6191	CD	ARG	136	-13.850	-71.388	172.275	1.00	30.26	D	C
	ATOM	6192	NE	ARG	136	-13.587	-72.664	171.601	1.00	34.44	D	N
	ATOM	6193	CZ	ARG	136	-14.415	-73.709	171.612	1.00	36.40	D	C
	ATOM	6194	NH1	ARG	136	-15.577	-73.662	172.266	1.00	37.87	D	N
55	ATOM	6195	NH2	ARG	136	-14.085	-74.805	170.954	1.00	39.01	D	N
	ATOM	6196	C	ARG	136	-14.594	-68.449	168.261	1.00	20.52	D	C
	ATOM	6197	O	ARG	136	-13.537	-67.886	168.529	1.00	20.05	D	O
	ATOM	6198	N	PRO	137	-15.287	-68.157	167.151	1.00	20.21	D	N

-276-

	ATOM	6199	CD	PRO	137	-16.587	-68.657	166.661	1.00	20.40	D	C
	ATOM	6200	CA	PRO	137	-14.745	-67.136	166.252	1.00	21.02	D	C
	ATOM	6201	CB	PRO	137	-15.646	-67.247	165.023	1.00	20.72	D	C
5	ATOM	6202	CG	PRO	137	-16.973	-67.612	165.628	1.00	21.45	D	C
	ATOM	6203	C	PRO	137	-14.806	-65.738	166.867	1.00	21.01	D	C
	ATOM	6204	O	PRO	137	-15.789	-65.373	167.509	1.00	20.39	D	O
	ATOM	6205	N	PRO	138	-13.735	-64.949	166.710	1.00	21.11	D	N
	ATOM	6206	CD	PRO	138	-12.375	-65.323	166.286	1.00	21.05	D	C
10	ATOM	6207	CA	PRO	138	-13.764	-63.593	167.272	1.00	21.01	D	C
	ATOM	6208	CB	PRO	138	-12.400	-63.036	166.890	1.00	21.60	D	C
	ATOM	6209	CG	PRO	138	-11.523	-64.269	166.967	1.00	22.95	D	C
	ATOM	6210	C	PRO	138	-14.914	-62.830	166.605	1.00	20.24	D	C
	ATOM	6211	O	PRO	138	-15.328	-63.174	165.490	1.00	17.44	D	O
15	ATOM	6212	N	ALA	139	-15.419	-61.804	167.289	1.00	19.19	D	N
	ATOM	6213	CA	ALA	139	-16.537	-60.991	166.804	1.00	17.76	D	C
	ATOM	6214	CB	ALA	139	-16.859	-59.892	167.827	1.00	17.06	D	C
	ATOM	6215	C	ALA	139	-16.346	-60.360	165.430	1.00	17.86	D	C
	ATOM	6216	O	ALA	139	-17.294	-60.281	164.645	1.00	17.93	D	O
20	ATOM	6217	N	HIS	140	-15.133	-59.906	165.130	1.00	17.55	D	N
	ATOM	6218	CA	HIS	140	-14.886	-59.266	163.842	1.00	16.71	D	C
	ATOM	6219	CB	HIS	140	-13.507	-58.578	163.825	1.00	16.46	D	C
	ATOM	6220	CG	HIS	140	-12.363	-59.501	163.533	1.00	15.67	D	C
	ATOM	6221	CD2	HIS	140	-11.736	-59.798	162.371	1.00	14.99	D	C
25	ATOM	6222	ND1	HIS	140	-11.745	-60.257	164.508	1.00	13.91	D	N
	ATOM	6223	CE1	HIS	140	-10.786	-60.979	163.956	1.00	14.59	D	C
	ATOM	6224	NE2	HIS	140	-10.759	-60.719	162.661	1.00	15.09	D	N
	ATOM	6225	C	HIS	140	-15.013	-60.212	162.650	1.00	16.75	D	C
	ATOM	6226	O	HIS	140	-15.105	-59.764	161.513	1.00	15.99	D	O
30	ATOM	6227	N	LEU	141	-15.033	-61.518	162.901	1.00	17.79	D	N
	ATOM	6228	CA	LEU	141	-15.158	-62.487	161.814	1.00	18.75	D	C
	ATOM	6229	CB	LEU	141	-14.682	-63.869	162.273	1.00	18.44	D	C
	ATOM	6230	CG	LEU	141	-13.186	-64.038	162.573	1.00	18.91	D	C
	ATOM	6231	CD1	LEU	141	-12.904	-65.504	162.883	1.00	17.51	D	C
35	ATOM	6232	CD2	LEU	141	-12.345	-63.588	161.362	1.00	17.97	D	C
	ATOM	6233	C	LEU	141	-16.588	-62.590	161.283	1.00	20.14	D	C
	ATOM	6234	O	LEU	141	-16.806	-63.055	160.167	1.00	19.48	D	O
	ATOM	6235	N	PHE	142	-17.565	-62.172	162.084	1.00	21.14	D	N
	ATOM	6236	CA	PHE	142	-18.950	-62.224	161.649	1.00	23.17	D	C
40	ATOM	6237	CB	PHE	142	-19.908	-62.041	162.837	1.00	22.30	D	C
	ATOM	6238	CG	PHE	142	-19.998	-63.249	163.726	1.00	22.33	D	C
	ATOM	6239	CD1	PHE	142	-19.018	-63.510	164.673	1.00	22.28	D	C
	ATOM	6240	CD2	PHE	142	-21.039	-64.158	163.578	1.00	22.17	D	C
	ATOM	6241	CE1	PHE	142	-19.073	-64.655	165.455	1.00	22.00	D	C
	ATOM	6242	CE2	PHE	142	-21.099	-65.301	164.353	1.00	20.89	D	C
45	ATOM	6243	CZ	PHE	142	-20.116	-65.550	165.293	1.00	21.02	D	C
	ATOM	6244	C	PHE	142	-19.229	-61.177	160.580	1.00	25.02	D	C
	ATOM	6245	O	PHE	142	-18.818	-60.018	160.692	1.00	24.19	D	O
	ATOM	6246	N	ILE	143	-19.924	-61.610	159.534	1.00	28.08	D	N
50	ATOM	6247	CA	ILE	143	-20.281	-60.755	158.410	1.00	31.14	D	C
	ATOM	6248	CB	ILE	143	-21.243	-61.528	157.446	1.00	32.88	D	C
	ATOM	6249	CG2	ILE	143	-22.689	-61.262	157.814	1.00	33.01	D	C
	ATOM	6250	CG1	ILE	143	-20.965	-61.152	155.986	1.00	34.33	D	C
	ATOM	6251	CD1	ILE	143	-21.350	-59.741	155.606	1.00	36.85	D	C
55	ATOM	6252	C	ILE	143	-20.929	-59.455	158.913	1.00	32.38	D	C
	ATOM	6253	O	ILE	143	-21.768	-59.473	159.820	1.00	31.70	D	O
	ATOM	6254	N	HIS	144	-20.503	-58.333	158.334	1.00	33.55	D	N
	ATOM	6255	CA	HIS	144	-21.008	-57.003	158.680	1.00	34.98	D	C
	ATOM	6256	CB	HIS	144	-22.543	-56.993	158.683	1.00	37.72	D	C

-277-

5	ATOM	6257	CG	HIS	144	-23.145	-57.259	157.339	1.00	40.12	D	C
	ATOM	6258	CD2	HIS	144	-24.003	-58.218	156.919	1.00	41.14	D	C
	ATOM	6259	ND1	HIS	144	-22.833	-56.510	156.224	1.00	41.50	D	N
	ATOM	6260	CE1	HIS	144	-23.470	-56.999	155.174	1.00	41.78	D	C
	ATOM	6261	NE2	HIS	144	-24.186	-58.036	155.569	1.00	42.04	D	N
10	ATOM	6262	C	HIS	144	-20.491	-56.424	159.990	1.00	34.54	D	C
	ATOM	6263	O	HIS	144	-20.892	-55.329	160.386	1.00	34.20	D	O
	ATOM	6264	N	HIS	145	-19.605	-57.147	160.666	1.00	33.54	D	N
	ATOM	6265	CA	HIS	145	-19.048	-56.650	161.916	1.00	32.95	D	C
	ATOM	6266	CB	HIS	145	-18.722	-57.816	162.865	1.00	32.61	D	C
15	ATOM	6267	CG	HIS	145	-18.476	-57.400	164.287	1.00	32.37	D	C
	ATOM	6268	CD2	HIS	145	-19.265	-57.477	165.386	1.00	32.00	D	C
	ATOM	6269	ND1	HIS	145	-17.300	-56.811	164.704	1.00	32.66	D	N
	ATOM	6270	CE1	HIS	145	-17.374	-56.542	165.995	1.00	31.20	D	C
	ATOM	6271	NE2	HIS	145	-18.557	-56.936	166.434	1.00	32.43	D	N
20	ATOM	6272	C	HIS	145	-17.788	-55.841	161.605	1.00	32.76	D	C
	ATOM	6273	O	HIS	145	-17.068	-56.117	160.647	1.00	32.46	D	O
	ATOM	6274	N	GLN	146	-17.559	-54.820	162.417	1.00	32.73	D	N
	ATOM	6275	CA	GLN	146	-16.411	-53.932	162.315	1.00	32.80	D	C
	ATOM	6276	CB	GLN	146	-16.542	-52.924	163.466	1.00	36.08	D	C
25	ATOM	6277	CG	GLN	146	-15.335	-52.084	163.823	1.00	40.75	D	C
	ATOM	6278	CD	GLN	146	-15.660	-51.061	164.913	1.00	42.71	D	C
	ATOM	6279	OE1	GLN	146	-14.828	-50.770	165.781	1.00	44.05	D	O
	ATOM	6280	NE2	GLN	146	-16.870	-50.503	164.862	1.00	42.83	D	N
	ATOM	6281	C	GLN	146	-15.087	-54.727	162.374	1.00	30.70	D	C
30	ATOM	6282	O	GLN	146	-14.985	-55.716	163.093	1.00	29.52	D	O
	ATOM	6283	N	PRO	147	-14.067	-54.307	161.599	1.00	29.06	D	N
	ATOM	6284	CD	PRO	147	-14.144	-53.170	160.666	1.00	29.28	D	C
	ATOM	6285	CA	PRO	147	-12.738	-54.946	161.532	1.00	27.41	D	C
	ATOM	6286	CB	PRO	147	-11.969	-54.050	160.559	1.00	27.81	D	C
35	ATOM	6287	CG	PRO	147	-13.042	-53.488	159.682	1.00	28.67	D	C
	ATOM	6288	C	PRO	147	-12.040	-55.020	162.894	1.00	25.53	D	C
	ATOM	6289	O	PRO	147	-12.434	-54.328	163.831	1.00	26.05	D	O
	ATOM	6290	N	LEU	148	-11.008	-55.854	163.009	1.00	23.12	D	N
	ATOM	6291	CA	LEU	148	-10.282	-55.979	164.280	1.00	21.13	D	C
40	ATOM	6292	CB	LEU	148	-9.302	-57.153	164.231	1.00	20.59	D	C
	ATOM	6293	CG	LEU	148	-8.531	-57.403	165.532	1.00	20.63	D	C
	ATOM	6294	CD1	LEU	148	-9.478	-57.969	166.595	1.00	18.94	D	C
	ATOM	6295	CD2	LEU	148	-7.384	-58.372	165.270	1.00	20.92	D	C
	ATOM	6296	C	LEU	148	-9.509	-54.687	164.547	1.00	19.93	D	C
45	ATOM	6297	O	LEU	148	-8.641	-54.304	163.766	1.00	19.73	D	O
	ATOM	6298	N	PRO	149	-9.815	-53.995	165.654	1.00	18.90	D	N
	ATOM	6299	CD	PRO	149	-10.844	-54.314	166.658	1.00	18.79	D	C
	ATOM	6300	CA	PRO	149	-9.129	-52.738	165.992	1.00	18.86	D	C
	ATOM	6301	CB	PRO	149	-9.726	-52.368	167.351	1.00	17.91	D	C
50	ATOM	6302	CG	PRO	149	-11.102	-52.954	167.290	1.00	18.09	D	C
	ATOM	6303	C	PRO	149	-7.608	-52.836	166.056	1.00	18.30	D	C
	ATOM	6304	O	PRO	149	-7.045	-53.894	166.310	1.00	18.17	D	O
	ATOM	6305	N	THR	150	-6.954	-51.706	165.837	1.00	19.06	D	N
	ATOM	6306	CA	THR	150	-5.509	-51.619	165.870	1.00	18.45	D	C
55	ATOM	6307	CB	THR	150	-5.060	-50.141	165.785	1.00	18.97	D	C
	ATOM	6308	OG1	THR	150	-5.334	-49.633	164.469	1.00	16.80	D	O
	ATOM	6309	CG2	THR	150	-3.574	-50.007	166.110	1.00	16.34	D	C
	ATOM	6310	C	THR	150	-4.875	-52.247	167.112	1.00	19.56	D	C
	ATOM	6311	O	THR	150	-3.923	-53.016	167.003	1.00	20.79	D	O
	ATOM	6312	N	LEU	151	-5.391	-51.928	168.292	1.00	19.20	D	N
	ATOM	6313	CA	LEU	151	-4.792	-52.451	169.518	1.00	19.49	D	C
	ATOM	6314	CB	LEU	151	-4.714	-51.338	170.579	1.00	19.37	D	C

-278-

5	ATOM	6315	CG	LEU	151	-3.833	-50.116	170.260	1.00	19.71	D	C
	ATOM	6316	CD1	LEU	151	-3.960	-49.078	171.376	1.00	19.45	D	C
	ATOM	6317	CD2	LEU	151	-2.384	-50.542	170.112	1.00	19.57	D	C
	ATOM	6318	C	LEU	151	-5.466	-53.680	170.124	1.00	19.39	D	C
	ATOM	6319	O	LEU	151	-5.067	-54.136	171.194	1.00	18.10	D	O
10	ATOM	6320	N	ALA	152	-6.480	-54.220	169.456	1.00	18.60	D	N
	ATOM	6321	CA	ALA	152	-7.162	-55.396	169.986	1.00	18.53	D	C
	ATOM	6322	CB	ALA	152	-8.407	-55.695	169.166	1.00	17.95	D	C
	ATOM	6323	C	ALA	152	-6.228	-56.605	169.980	1.00	18.77	D	C
	ATOM	6324	O	ALA	152	-5.473	-56.815	169.034	1.00	18.21	D	O
15	ATOM	6325	N	PRO	153	-6.256	-57.413	171.050	1.00	18.94	D	N
	ATOM	6326	CD	PRO	153	-7.013	-57.266	172.306	1.00	18.91	D	C
	ATOM	6327	CA	PRO	153	-5.378	-58.592	171.086	1.00	19.14	D	C
	ATOM	6328	CB	PRO	153	-5.693	-59.220	172.442	1.00	19.09	D	C
	ATOM	6329	CG	PRO	153	-6.151	-58.035	173.283	1.00	20.56	D	C
20	ATOM	6330	C	PRO	153	-5.715	-59.549	169.939	1.00	18.81	D	C
	ATOM	6331	O	PRO	153	-6.886	-59.704	169.589	1.00	17.99	D	O
	ATOM	6332	N	VAL	154	-4.701	-60.179	169.350	1.00	18.43	D	N
	ATOM	6333	CA	VAL	154	-4.952	-61.139	168.269	1.00	18.36	D	C
	ATOM	6334	CB	VAL	154	-3.839	-61.104	167.166	1.00	18.03	D	C
25	ATOM	6335	CG1	VAL	154	-3.757	-59.717	166.551	1.00	19.77	D	C
	ATOM	6336	CG2	VAL	154	-2.499	-61.511	167.747	1.00	17.94	D	C
	ATOM	6337	C	VAL	154	-5.079	-62.584	168.787	1.00	17.46	D	C
	ATOM	6338	O	VAL	154	-5.477	-63.476	168.047	1.00	16.70	D	O
	ATOM	6339	N	LEU	155	-4.740	-62.815	170.053	1.00	17.73	D	N
30	ATOM	6340	CA	LEU	155	-4.834	-64.160	170.637	1.00	18.30	D	C
	ATOM	6341	CB	LEU	155	-4.640	-64.091	172.156	1.00	18.87	D	C
	ATOM	6342	CG	LEU	155	-4.657	-65.402	172.949	1.00	18.81	D	C
	ATOM	6343	CD1	LEU	155	-3.620	-66.374	172.393	1.00	18.11	D	C
	ATOM	6344	CD2	LEU	155	-4.375	-65.092	174.426	1.00	19.81	D	C
35	ATOM	6345	C	LEU	155	-6.144	-64.897	170.305	1.00	18.45	D	C
	ATOM	6346	O	LEU	155	-6.114	-66.057	169.897	1.00	19.26	D	O
	ATOM	6347	N	PRO	156	-7.310	-64.243	170.480	1.00	18.25	D	N
	ATOM	6348	CD	PRO	156	-7.607	-62.946	171.115	1.00	17.28	D	C
	ATOM	6349	CA	PRO	156	-8.555	-64.955	170.153	1.00	17.77	D	C
40	ATOM	6350	CB	PRO	156	-9.632	-63.899	170.409	1.00	17.59	D	C
	ATOM	6351	CG	PRO	156	-9.054	-63.126	171.560	1.00	17.51	D	C
	ATOM	6352	C	PRO	156	-8.576	-65.479	168.714	1.00	17.24	D	C
	ATOM	6353	O	PRO	156	-9.029	-66.595	168.458	1.00	16.32	D	O
	ATOM	6354	N	LEU	157	-8.086	-64.670	167.780	1.00	16.35	D	N
45	ATOM	6355	CA	LEU	157	-8.034	-65.057	166.374	1.00	15.67	D	C
	ATOM	6356	CB	LEU	157	-7.649	-63.855	165.510	1.00	15.48	D	C
	ATOM	6357	CG	LEU	157	-7.507	-64.123	164.007	1.00	14.81	D	C
	ATOM	6358	CD1	LEU	157	-8.827	-64.622	163.411	1.00	13.61	D	C
	ATOM	6359	CD2	LEU	157	-7.078	-62.837	163.337	1.00	14.21	D	C
50	ATOM	6360	C	LEU	157	-7.025	-66.186	166.151	1.00	15.16	D	C
	ATOM	6361	O	LEU	157	-7.294	-67.126	165.405	1.00	14.60	D	O
	ATOM	6362	N	VAL	158	-5.862	-66.081	166.788	1.00	14.93	D	N
	ATOM	6363	CA	VAL	158	-4.822	-67.107	166.677	1.00	16.52	D	C
	ATOM	6364	CB	VAL	158	-3.546	-66.699	167.478	1.00	17.32	D	C
55	ATOM	6365	CG1	VAL	158	-2.554	-67.865	167.538	1.00	16.08	D	C
	ATOM	6366	CG2	VAL	158	-2.884	-65.489	166.825	1.00	15.99	D	C
	ATOM	6367	C	VAL	158	-5.343	-68.452	167.213	1.00	16.29	D	C
	ATOM	6368	O	VAL	158	-5.129	-69.505	166.604	1.00	14.70	D	O
	ATOM	6369	N	THR	159	-6.031	-68.408	168.350	1.00	16.12	D	N
	ATOM	6370	CA	THR	159	-6.583	-69.619	168.959	1.00	17.65	D	C
	ATOM	6371	CB	THR	159	-7.160	-69.322	170.352	1.00	17.07	D	C
	ATOM	6372	OG1	THR	159	-6.190	-68.592	171.109	1.00	16.57	D	O

-279-

	ATOM	6373	CG2	THR	159	-7.501	-70.626	171.094	1.00	17.20	D	C
	ATOM	6374	C	THR	159	-7.680	-70.194	168.063	1.00	17.34	D	C
	ATOM	6375	O	THR	159	-7.794	-71.409	167.908	1.00	17.77	D	O
5	ATOM	6376	N	HIS	160	-8.486	-69.315	167.478	1.00	16.89	D	N
	ATOM	6377	CA	HIS	160	-9.541	-69.738	166.567	1.00	16.98	D	C
	ATOM	6378	CB	HIS	160	-10.363	-68.539	166.103	1.00	16.02	D	C
	ATOM	6379	CG	HIS	160	-11.374	-68.886	165.058	1.00	16.63	D	C
	ATOM	6380	CD2	HIS	160	-11.450	-68.560	163.746	1.00	16.70	D	C
10	ATOM	6381	ND1	HIS	160	-12.451	-69.709	165.312	1.00	15.58	D	N
	ATOM	6382	CE1	HIS	160	-13.146	-69.873	164.200	1.00	16.17	D	C
	ATOM	6383	NE2	HIS	160	-12.560	-69.187	163.235	1.00	15.22	D	N
	ATOM	6384	C	HIS	160	-8.933	-70.440	165.338	1.00	16.47	D	C
	ATOM	6385	O	HIS	160	-9.446	-71.459	164.881	1.00	15.93	D	O
15	ATOM	6386	N	PHE	161	-7.855	-69.876	164.795	1.00	16.05	D	N
	ATOM	6387	CA	PHE	161	-7.186	-70.473	163.645	1.00	16.40	D	C
	ATOM	6388	CB	PHE	161	-6.057	-69.564	163.125	1.00	15.95	D	C
	ATOM	6389	CG	PHE	161	-6.516	-68.474	162.172	1.00	15.49	D	C
	ATOM	6390	CD1	PHE	161	-7.819	-68.444	161.679	1.00	15.45	D	C
20	ATOM	6391	CD2	PHE	161	-5.620	-67.496	161.739	1.00	15.30	D	C
	ATOM	6392	CE1	PHE	161	-8.228	-67.458	160.763	1.00	14.86	D	C
	ATOM	6393	CE2	PHE	161	-6.012	-66.506	160.826	1.00	15.33	D	C
	ATOM	6394	CZ	PHE	161	-7.323	-66.487	160.338	1.00	14.34	D	C
	ATOM	6395	C	PHE	161	-6.615	-71.833	164.066	1.00	16.58	D	C
25	ATOM	6396	O	PHE	161	-6.801	-72.830	163.377	1.00	16.53	D	O
	ATOM	6397	N	ALA	162	-5.926	-71.876	165.199	1.00	16.50	D	N
	ATOM	6398	CA	ALA	162	-5.368	-73.132	165.687	1.00	16.70	D	C
	ATOM	6399	CB	ALA	162	-4.745	-72.938	167.075	1.00	15.50	D	C
	ATOM	6400	C	ALA	162	-6.462	-74.198	165.750	1.00	16.99	D	C
30	ATOM	6401	O	ALA	162	-6.274	-75.310	165.263	1.00	16.57	D	O
	ATOM	6402	N	ASP	163	-7.610	-73.848	166.329	1.00	16.55	D	N
	ATOM	6403	CA	ASP	163	-8.711	-74.794	166.463	1.00	17.27	D	C
	ATOM	6404	CB	ASP	163	-9.759	-74.246	167.434	1.00	18.34	D	C
	ATOM	6405	CG	ASP	163	-9.238	-74.153	168.853	1.00	20.38	D	C
35	ATOM	6406	OD1	ASP	163	-9.950	-73.586	169.710	1.00	21.00	D	O
	ATOM	6407	OD2	ASP	163	-8.117	-74.652	169.109	1.00	19.55	D	O
	ATOM	6408	C	ASP	163	-9.388	-75.244	165.168	1.00	16.59	D	C
	ATOM	6409	O	ASP	163	-9.773	-76.408	165.054	1.00	14.65	D	O
	ATOM	6410	N	ILE	164	-9.561	-74.351	164.196	1.00	15.61	D	N
40	ATOM	6411	CA	ILE	164	-10.178	-74.802	162.955	1.00	15.63	D	C
	ATOM	6412	CB	ILE	164	-10.877	-73.655	162.151	1.00	14.12	D	C
	ATOM	6413	CG2	ILE	164	-11.951	-73.003	163.018	1.00	15.01	D	C
	ATOM	6414	CG1	ILE	164	-9.857	-72.630	161.666	1.00	14.02	D	C
	ATOM	6415	CD1	ILE	164	-10.461	-71.562	160.759	1.00	12.25	D	C
45	ATOM	6416	C	ILE	164	-9.135	-75.494	162.081	1.00	16.00	D	C
	ATOM	6417	O	ILE	164	-9.486	-76.288	161.215	1.00	16.41	D	O
	ATOM	6418	N	ASN	165	-7.855	-75.194	162.300	1.00	15.80	D	N
	ATOM	6419	CA	ASN	165	-6.793	-75.851	161.542	1.00	17.21	D	C
	ATOM	6420	CB	ASN	165	-5.421	-75.221	161.814	1.00	16.55	D	C
50	ATOM	6421	CG	ASN	165	-5.211	-73.916	161.068	1.00	17.71	D	C
	ATOM	6422	OD1	ASN	165	-5.933	-73.603	160.122	1.00	16.40	D	O
	ATOM	6423	ND2	ASN	165	-4.198	-73.156	161.482	1.00	16.80	D	N
	ATOM	6424	C	ASN	165	-6.763	-77.315	161.990	1.00	17.61	D	C
	ATOM	6425	O	ASN	165	-6.618	-78.222	161.174	1.00	17.26	D	O
55	ATOM	6426	N	THR	166	-6.883	-77.539	163.297	1.00	17.61	D	N
	ATOM	6427	CA	THR	166	-6.893	-78.897	163.818	1.00	17.94	D	C
	ATOM	6428	CB	THR	166	-6.821	-78.887	165.355	1.00	18.82	D	C
	ATOM	6429	OG1	THR	166	-5.537	-78.387	165.748	1.00	19.08	D	O
	ATOM	6430	CG2	THR	166	-7.015	-80.301	165.927	1.00	16.51	D	C

-280-

5	ATOM	6431	C	THR	166	-8.164	-79.604	163.343	1.00	18.00	D	C
	ATOM	6432	O	THR	166	-8.111	-80.734	162.869	1.00	18.63	D	O
	ATOM	6433	N	PHE	167	-9.304	-78.930	163.462	1.00	17.77	D	N
	ATOM	6434	CA	PHE	167	-10.569	-79.496	163.012	1.00	18.33	D	C
	ATOM	6435	CB	PHE	167	-11.700	-78.473	163.157	1.00	18.78	D	C
10	ATOM	6436	CG	PHE	167	-12.945	-78.825	162.382	1.00	19.22	D	C
	ATOM	6437	CD1	PHE	167	-13.727	-79.923	162.743	1.00	19.14	D	C
	ATOM	6438	CD2	PHE	167	-13.343	-78.046	161.294	1.00	19.37	D	C
	ATOM	6439	CE1	PHE	167	-14.892	-80.236	162.036	1.00	18.14	D	C
	ATOM	6440	CE2	PHE	167	-14.499	-78.348	160.583	1.00	19.96	D	C
15	ATOM	6441	CZ	PHE	167	-15.279	-79.447	160.956	1.00	20.10	D	C
	ATOM	6442	C	PHE	167	-10.469	-79.931	161.550	1.00	18.30	D	C
	ATOM	6443	O	PHE	167	-10.862	-81.046	161.211	1.00	18.49	D	O
	ATOM	6444	N	MET	168	-9.935	-79.058	160.694	1.00	17.27	D	N
	ATOM	6445	CA	MET	168	-9.804	-79.365	159.269	1.00	17.47	D	C
20	ATOM	6446	CB	MET	168	-9.301	-78.138	158.484	1.00	17.11	D	C
	ATOM	6447	CG	MET	168	-10.388	-77.099	158.163	1.00	17.30	D	C
	ATOM	6448	SD	MET	168	-9.818	-75.771	157.061	1.00	15.92	D	S
	ATOM	6449	CE	MET	168	-8.921	-74.718	158.216	1.00	15.99	D	C
	ATOM	6450	C	MET	168	-8.921	-80.572	158.949	1.00	16.51	D	C
25	ATOM	6451	O	MET	168	-9.292	-81.405	158.120	1.00	15.80	D	O
	ATOM	6452	N	VAL	169	-7.757	-80.672	159.582	1.00	16.26	D	N
	ATOM	6453	CA	VAL	169	-6.875	-81.814	159.313	1.00	17.34	D	C
	ATOM	6454	CB	VAL	169	-5.523	-81.673	160.042	1.00	17.83	D	C
	ATOM	6455	CG1	VAL	169	-4.681	-82.927	159.813	1.00	18.06	D	C
30	ATOM	6456	CG2	VAL	169	-4.786	-80.443	159.527	1.00	17.43	D	C
	ATOM	6457	C	VAL	169	-7.540	-83.129	159.739	1.00	17.64	D	C
	ATOM	6458	O	VAL	169	-7.398	-84.163	159.076	1.00	16.56	D	O
	ATOM	6459	N	LEU	170	-8.271	-83.093	160.847	1.00	17.79	D	N
	ATOM	6460	CA	LEU	170	-8.966	-84.285	161.302	1.00	19.01	D	C
35	ATOM	6461	CB	LEU	170	-9.624	-84.031	162.656	1.00	20.40	D	C
	ATOM	6462	CG	LEU	170	-8.588	-83.884	163.770	1.00	22.26	D	C
	ATOM	6463	CD1	LEU	170	-9.244	-83.352	165.038	1.00	23.26	D	C
	ATOM	6464	CD2	LEU	170	-7.930	-85.239	164.010	1.00	23.21	D	C
	ATOM	6465	C	LEU	170	-10.008	-84.677	160.258	1.00	19.01	D	C
40	ATOM	6466	O	LEU	170	-10.235	-85.865	160.021	1.00	19.62	D	O
	ATOM	6467	N	GLN	171	-10.628	-83.684	159.621	1.00	18.39	D	N
	ATOM	6468	CA	GLN	171	-11.624	-83.966	158.591	1.00	19.08	D	C
	ATOM	6469	CB	GLN	171	-12.392	-82.695	158.225	1.00	19.14	D	C
	ATOM	6470	CG	GLN	171	-13.319	-82.222	159.342	1.00	20.31	D	C
45	ATOM	6471	CD	GLN	171	-14.329	-83.293	159.744	1.00	20.59	D	C
	ATOM	6472	OE1	GLN	171	-15.207	-83.671	158.960	1.00	23.53	D	O
	ATOM	6473	NE2	GLN	171	-14.202	-83.792	160.955	1.00	19.36	D	N
	ATOM	6474	C	GLN	171	-10.989	-84.594	157.346	1.00	19.36	D	C
	ATOM	6475	O	GLN	171	-11.572	-85.491	156.736	1.00	18.90	D	O
50	ATOM	6476	N	VAL	172	-9.801	-84.124	156.968	1.00	18.78	D	N
	ATOM	6477	CA	VAL	172	-9.100	-84.689	155.817	1.00	19.25	D	C
	ATOM	6478	CB	VAL	172	-7.753	-83.960	155.559	1.00	19.23	D	C
	ATOM	6479	CG1	VAL	172	-6.918	-84.732	154.527	1.00	17.92	D	C
	ATOM	6480	CG2	VAL	172	-8.017	-82.547	155.063	1.00	18.09	D	C
55	ATOM	6481	C	VAL	172	-8.822	-86.178	156.097	1.00	19.25	D	C
	ATOM	6482	O	VAL	172	-8.956	-87.020	155.213	1.00	17.74	D	O
	ATOM	6483	N	ILE	173	-8.436	-86.484	157.333	1.00	19.42	D	N
	ATOM	6484	CA	ILE	173	-8.154	-87.857	157.748	1.00	20.65	D	C
	ATOM	6485	CB	ILE	173	-7.679	-87.898	159.227	1.00	21.20	D	C
	ATOM	6486	CG2	ILE	173	-7.666	-89.341	159.756	1.00	20.73	D	C
	ATOM	6487	CG1	ILE	173	-6.290	-87.266	159.332	1.00	19.71	D	C
	ATOM	6488	CD1	ILE	173	-5.807	-87.079	160.744	1.00	20.26	D	C

-281-

	ATOM	6489	C	ILE	173	-9.400	-88.727	157.575	1.00	21.22	D	C
	ATOM	6490	O	ILE	173	-9.313	-89.847	157.081	1.00	21.19	D	O
	ATOM	6491	N	LYS	174	-10.557	-88.211	157.982	1.00	21.41	D	N
5	ATOM	6492	CA	LYS	174	-11.808	-88.946	157.835	1.00	22.16	D	C
	ATOM	6493	CB	LYS	174	-12.933	-88.231	158.599	1.00	23.61	D	C
	ATOM	6494	CG	LYS	174	-12.720	-88.228	160.119	1.00	25.13	D	C
	ATOM	6495	CD	LYS	174	-13.770	-87.422	160.870	1.00	26.92	D	C
	ATOM	6496	CE	LYS	174	-15.122	-88.112	160.854	1.00	30.21	D	C
10	ATOM	6497	NZ	LYS	174	-16.122	-87.399	161.705	1.00	31.50	D	N
	ATOM	6498	C	LYS	174	-12.156	-89.082	156.348	1.00	22.88	D	C
	ATOM	6499	O	LYS	174	-12.806	-90.045	155.932	1.00	21.83	D	O
	ATOM	6500	N	PHE	175	-11.715	-88.112	155.548	1.00	23.02	D	N
	ATOM	6501	CA	PHE	175	-11.944	-88.125	154.107	1.00	23.18	D	C
15	ATOM	6502	CB	PHE	175	-11.506	-86.785	153.498	1.00	22.95	D	C
	ATOM	6503	CG	PHE	175	-11.194	-86.842	152.024	1.00	22.60	D	C
	ATOM	6504	CD1	PHE	175	-12.199	-87.063	151.086	1.00	21.67	D	C
	ATOM	6505	CD2	PHE	175	-9.893	-86.636	151.575	1.00	22.02	D	C
	ATOM	6506	CE1	PHE	175	-11.910	-87.074	149.719	1.00	22.60	D	C
20	ATOM	6507	CE2	PHE	175	-9.593	-86.645	150.215	1.00	22.13	D	C
	ATOM	6508	CZ	PHE	175	-10.602	-86.864	149.284	1.00	22.45	D	C
	ATOM	6509	C	PHE	175	-11.154	-89.268	153.479	1.00	23.77	D	C
	ATOM	6510	O	PHE	175	-11.702	-90.070	152.725	1.00	23.33	D	O
	ATOM	6511	N	THR	176	-9.867	-89.346	153.805	1.00	24.37	D	N
25	ATOM	6512	CA	THR	176	-9.006	-90.381	153.248	1.00	25.40	D	C
	ATOM	6513	CB	THR	176	-7.519	-90.090	153.542	1.00	25.42	D	C
	ATOM	6514	OG1	THR	176	-7.317	-89.986	154.956	1.00	26.76	D	O
	ATOM	6515	CG2	THR	176	-7.094	-88.782	152.878	1.00	25.58	D	C
	ATOM	6516	C	THR	176	-9.348	-91.792	153.733	1.00	26.23	D	C
30	ATOM	6517	O	THR	176	-9.105	-92.765	153.012	1.00	26.27	D	O
	ATOM	6518	N	LYS	177	-9.915	-91.908	154.935	1.00	26.44	D	N
	ATOM	6519	CA	LYS	177	-10.278	-93.224	155.453	1.00	27.74	D	C
	ATOM	6520	CB	LYS	177	-10.871	-93.143	156.867	1.00	27.72	D	C
	ATOM	6521	CG	LYS	177	-11.345	-94.527	157.354	1.00	28.98	D	C
35	ATOM	6522	CD	LYS	177	-11.991	-94.514	158.723	1.00	28.59	D	C
	ATOM	6523	CE	LYS	177	-12.497	-95.914	159.106	1.00	28.79	D	C
	ATOM	6524	NZ	LYS	177	-13.703	-96.370	158.341	1.00	27.25	D	N
	ATOM	6525	C	LYS	177	-11.287	-93.906	154.546	1.00	27.56	D	C
	ATOM	6526	O	LYS	177	-11.251	-95.124	154.381	1.00	27.25	D	O
40	ATOM	6527	N	ASP	178	-12.183	-93.111	153.966	1.00	27.88	D	N
	ATOM	6528	CA	ASP	178	-13.218	-93.616	153.069	1.00	28.74	D	C
	ATOM	6529	CB	ASP	178	-14.388	-92.627	153.006	1.00	29.09	D	C
	ATOM	6530	CG	ASP	178	-15.247	-92.647	154.258	1.00	30.01	D	C
	ATOM	6531	OD1	ASP	178	-14.983	-93.459	155.168	1.00	30.64	D	O
45	ATOM	6532	OD2	ASP	178	-16.202	-91.851	154.327	1.00	30.67	D	O
	ATOM	6533	C	ASP	178	-12.736	-93.894	151.644	1.00	28.80	D	C
	ATOM	6534	O	ASP	178	-13.556	-94.076	150.743	1.00	29.46	D	O
	ATOM	6535	N	LEU	179	-11.420	-93.910	151.434	1.00	28.53	D	N
	ATOM	6536	CA	LEU	179	-10.854	-94.176	150.112	1.00	27.98	D	C
50	ATOM	6537	CB	LEU	179	-9.889	-93.062	149.696	1.00	27.06	D	C
	ATOM	6538	CG	LEU	179	-10.423	-91.626	149.737	1.00	26.57	D	C
	ATOM	6539	CD1	LEU	179	-9.379	-90.688	149.145	1.00	26.43	D	C
	ATOM	6540	CD2	LEU	179	-11.718	-91.526	148.959	1.00	25.98	D	C
	ATOM	6541	C	LEU	179	-10.110	-95.498	150.185	1.00	28.10	D	C
55	ATOM	6542	O	LEU	179	-8.988	-95.562	150.683	1.00	27.56	D	O
	ATOM	6543	N	PRO	180	-10.732	-96.576	149.682	1.00	28.79	D	N
	ATOM	6544	CD	PRO	180	-12.040	-96.587	148.999	1.00	28.88	D	C
	ATOM	6545	CA	PRO	180	-10.141	-97.917	149.691	1.00	29.36	D	C
	ATOM	6546	CB	PRO	180	-11.089	-98.713	148.793	1.00	29.68	D	C

-282-

5	ATOM	6547	CG	PRO	180	-12.420	-98.052	149.056	1.00	28.81	D	C
	ATOM	6548	C	PRO	180	-8.691	-97.991	149.223	1.00	29.88	D	C
	ATOM	6549	O	PRO	180	-7.838	-98.543	149.918	1.00	29.69	D	O
	ATOM	6550	N	VAL	181	-8.399	-97.429	148.055	1.00	30.49	D	N
	ATOM	6551	CA	VAL	181	-7.036	-97.489	147.554	1.00	31.05	D	C
10	ATOM	6552	CB	VAL	181	-6.943	-96.959	146.105	1.00	32.32	D	C
	ATOM	6553	CG1	VAL	181	-7.329	-95.478	146.032	1.00	33.43	D	C
	ATOM	6554	CG2	VAL	181	-5.545	-97.204	145.582	1.00	33.81	D	C
	ATOM	6555	C	VAL	181	-6.030	-96.777	148.462	1.00	30.44	D	C
	ATOM	6556	O	VAL	181	-4.866	-97.172	148.533	1.00	31.06	D	O
15	ATOM	6557	N	PHE	182	-6.469	-95.732	149.160	1.00	29.10	D	N
	ATOM	6558	CA	PHE	182	-5.587	-95.039	150.098	1.00	27.62	D	C
	ATOM	6559	CB	PHE	182	-6.256	-93.762	150.616	1.00	26.73	D	C
	ATOM	6560	CG	PHE	182	-5.440	-93.014	151.645	1.00	26.35	D	C
	ATOM	6561	CD1	PHE	182	-4.393	-92.177	151.256	1.00	26.19	D	C
20	ATOM	6562	CD2	PHE	182	-5.726	-93.136	153.002	1.00	25.82	D	C
	ATOM	6563	CE1	PHE	182	-3.645	-91.471	152.204	1.00	25.18	D	C
	ATOM	6564	CE2	PHE	182	-4.983	-92.433	153.960	1.00	25.85	D	C
	ATOM	6565	CZ	PHE	182	-3.942	-91.599	153.558	1.00	24.75	D	C
	ATOM	6566	C	PHE	182	-5.347	-96.000	151.273	1.00	27.26	D	C
25	ATOM	6567	O	PHE	182	-4.218	-96.201	151.707	1.00	25.52	D	O
	ATOM	6568	N	ARG	183	-6.426	-96.599	151.772	1.00	27.61	D	N
	ATOM	6569	CA	ARG	183	-6.348	-97.535	152.900	1.00	29.82	D	C
	ATOM	6570	CB	ARG	183	-7.751	-97.955	153.342	1.00	29.81	D	C
	ATOM	6571	CG	ARG	183	-8.610	-96.819	153.834	1.00	30.04	D	C
30	ATOM	6572	CD	ARG	183	-8.065	-96.222	155.126	1.00	31.16	D	C
	ATOM	6573	NE	ARG	183	-8.007	-97.174	156.241	1.00	32.26	D	N
	ATOM	6574	CZ	ARG	183	-9.048	-97.832	156.752	1.00	33.84	D	C
	ATOM	6575	NH1	ARG	183	-10.271	-97.670	156.256	1.00	34.26	D	N
	ATOM	6576	NH2	ARG	183	-8.870	-98.641	157.788	1.00	32.25	D	N
35	ATOM	6577	C	ARG	183	-5.538	-98.791	152.611	1.00	30.35	D	C
	ATOM	6578	O	ARG	183	-5.025	-99.428	153.536	1.00	30.29	D	O
	ATOM	6579	N	SER	184	-5.436	-99.155	151.335	1.00	30.53	D	N
	ATOM	6580	CA	SER	184	-4.680	-100.341	150.937	1.00	31.20	D	C
	ATOM	6581	CB	SER	184	-4.960	-100.687	149.472	1.00	31.90	D	C
40	ATOM	6582	OG	SER	184	-6.311	-101.079	149.299	1.00	34.38	D	O
	ATOM	6583	C	SER	184	-3.187	-100.149	151.129	1.00	31.02	D	C
	ATOM	6584	O	SER	184	-2.440	-101.119	151.218	1.00	31.50	D	O
	ATOM	6585	N	LEU	185	-2.752	-98.894	151.185	1.00	30.38	D	N
	ATOM	6586	CA	LEU	185	-1.340	-98.580	151.369	1.00	30.35	D	C
45	ATOM	6587	CB	LEU	185	-1.076	-97.105	151.031	1.00	30.07	D	C
	ATOM	6588	CG	LEU	185	-1.534	-96.535	149.683	1.00	30.04	D	C
	ATOM	6589	CD1	LEU	185	-1.345	-95.013	149.690	1.00	28.56	D	C
	ATOM	6590	CD2	LEU	185	-0.748	-97.180	148.546	1.00	28.92	D	C
	ATOM	6591	C	LEU	185	-0.974	-98.817	152.831	1.00	30.64	D	C
50	ATOM	6592	O	LEU	185	-1.848	-98.832	153.696	1.00	30.76	D	O
	ATOM	6593	N	PRO	186	0.320	-99.018	153.125	1.00	31.27	D	N
	ATOM	6594	CD	PRO	186	1.483	-99.091	152.224	1.00	31.66	D	C
	ATOM	6595	CA	PRO	186	0.724	-99.235	154.515	1.00	31.60	D	C
	ATOM	6596	CB	PRO	186	2.220	-99.522	154.401	1.00	31.16	D	C
55	ATOM	6597	CG	PRO	186	2.620	-98.801	153.164	1.00	32.29	D	C
	ATOM	6598	C	PRO	186	0.419	-97.956	155.299	1.00	31.66	D	C
	ATOM	6599	O	PRO	186	0.609	-96.855	154.791	1.00	31.55	D	O
	ATOM	6600	N	ILE	187	-0.054	-98.106	156.531	1.00	31.45	D	N
	ATOM	6601	CA	ILE	187	-0.425	-96.959	157.351	1.00	31.05	D	C
	ATOM	6602	CB	ILE	187	-0.893	-97.417	158.766	1.00	29.97	D	C
	ATOM	6603	CG2	ILE	187	0.292	-97.909	159.591	1.00	29.23	D	C
	ATOM	6604	CG1	ILE	187	-1.606	-96.264	159.476	1.00	28.40	D	C

-283-

	ATOM	6605	CD1	ILE	187	-2.382	-96.690	160.706	1.00	27.64	D	C
	ATOM	6606	C	ILE	187	0.637	-95.861	157.485	1.00	31.86	D	C
	ATOM	6607	O	ILE	187	0.290	-94.683	157.625	1.00	31.41	D	O
5	ATOM	6608	N	GLU	188	1.917	-96.220	157.429	1.00	32.22	D	N
	ATOM	6609	CA	GLU	188	2.959	-95.207	157.553	1.00	33.67	D	C
	ATOM	6610	CB	GLU	188	4.325	-95.847	157.811	1.00	35.42	D	C
	ATOM	6611	CG	GLU	188	4.900	-96.637	156.663	1.00	38.74	D	C
	ATOM	6612	CD	GLU	188	6.331	-97.046	156.936	1.00	41.52	D	C
10	ATOM	6613	OE1	GLU	188	7.174	-96.137	157.118	1.00	42.54	D	O
	ATOM	6614	OE2	GLU	188	6.609	-98.267	156.974	1.00	42.40	D	O
	ATOM	6615	C	GLU	188	3.013	-94.324	156.307	1.00	33.32	D	C
	ATOM	6616	O	GLU	188	3.398	-93.158	156.381	1.00	33.14	D	O
	ATOM	6617	N	ASP	189	2.638	-94.888	155.163	1.00	32.68	D	N
15	ATOM	6618	CA	ASP	189	2.596	-94.130	153.921	1.00	32.83	D	C
	ATOM	6619	CB	ASP	189	2.505	-95.072	152.713	1.00	35.38	D	C
	ATOM	6620	CG	ASP	189	3.800	-95.828	152.465	1.00	37.57	D	C
	ATOM	6621	OD1	ASP	189	4.261	-96.542	153.384	1.00	40.86	D	O
	ATOM	6622	OD2	ASP	189	4.358	-95.705	151.354	1.00	37.64	D	O
20	ATOM	6623	C	ASP	189	1.362	-93.238	153.986	1.00	30.96	D	C
	ATOM	6624	O	ASP	189	1.407	-92.078	153.588	1.00	30.94	D	O
	ATOM	6625	N	GLN	190	0.262	-93.786	154.494	1.00	29.38	D	N
	ATOM	6626	CA	GLN	190	-0.973	-93.024	154.632	1.00	28.01	D	C
	ATOM	6627	CB	GLN	190	-2.046	-93.857	155.350	1.00	28.17	D	C
25	ATOM	6628	CG	GLN	190	-2.416	-95.171	154.661	1.00	28.90	D	C
	ATOM	6629	CD	GLN	190	-3.592	-95.899	155.323	1.00	29.16	D	C
	ATOM	6630	OE1	GLN	190	-3.808	-97.093	155.094	1.00	29.27	D	O
	ATOM	6631	NE2	GLN	190	-4.359	-95.180	156.130	1.00	28.27	D	N
	ATOM	6632	C	GLN	190	-0.675	-91.765	155.447	1.00	27.34	D	C
30	ATOM	6633	O	GLN	190	-1.122	-90.667	155.110	1.00	25.56	D	O
	ATOM	6634	N	ILE	191	0.089	-91.935	156.523	1.00	26.72	D	N
	ATOM	6635	CA	ILE	191	0.455	-90.823	157.389	1.00	26.98	D	C
	ATOM	6636	CB	ILE	191	1.106	-91.337	158.693	1.00	27.03	D	C
	ATOM	6637	CG2	ILE	191	1.671	-90.168	159.487	1.00	26.61	D	C
35	ATOM	6638	CG1	ILE	191	0.066	-92.108	159.520	1.00	26.71	D	C
	ATOM	6639	CD1	ILE	191	0.645	-92.862	160.693	1.00	27.05	D	C
	ATOM	6640	C	ILE	191	1.396	-89.835	156.690	1.00	26.93	D	C
	ATOM	6641	O	ILE	191	1.261	-88.624	156.859	1.00	25.97	D	O
	ATOM	6642	N	SER	192	2.343	-90.348	155.907	1.00	25.82	D	N
40	ATOM	6643	CA	SER	192	3.270	-89.486	155.183	1.00	26.80	D	C
	ATOM	6644	CB	SER	192	4.338	-90.325	154.473	1.00	27.15	D	C
	ATOM	6645	OG	SER	192	5.203	-90.939	155.415	1.00	29.76	D	O
	ATOM	6646	C	SER	192	2.531	-88.623	154.154	1.00	25.97	D	C
	ATOM	6647	O	SER	192	2.788	-87.425	154.037	1.00	25.52	D	O
45	ATOM	6648	N	LEU	193	1.621	-89.238	153.407	1.00	24.97	D	N
	ATOM	6649	CA	LEU	193	0.857	-88.516	152.402	1.00	24.60	D	C
	ATOM	6650	CB	LEU	193	0.061	-89.495	151.539	1.00	24.47	D	C
	ATOM	6651	CG	LEU	193	0.866	-90.473	150.667	1.00	25.09	D	C
	ATOM	6652	CD1	LEU	193	-0.091	-91.410	149.936	1.00	21.73	D	C
50	ATOM	6653	CD2	LEU	193	1.740	-89.688	149.673	1.00	24.35	D	C
	ATOM	6654	C	LEU	193	-0.088	-87.488	153.032	1.00	24.39	D	C
	ATOM	6655	O	LEU	193	-0.296	-86.410	152.476	1.00	23.01	D	O
	ATOM	6656	N	LEU	194	-0.667	-87.824	154.181	1.00	24.06	D	N
	ATOM	6657	CA	LEU	194	-1.575	-86.905	154.862	1.00	24.67	D	C
	ATOM	6658	CB	LEU	194	-2.283	-87.624	156.014	1.00	24.98	D	C
55	ATOM	6659	CG	LEU	194	-3.801	-87.862	155.880	1.00	27.03	D	C
	ATOM	6660	CD1	LEU	194	-4.556	-86.572	156.161	1.00	27.79	D	C
	ATOM	6661	CD2	LEU	194	-4.148	-88.367	154.492	1.00	28.80	D	C
	ATOM	6662	C	LEU	194	-0.766	-85.711	155.375	1.00	24.96	D	C

-284-

5	ATOM	6663	O	LEU	194	-1.173	-84.559	155.227	1.00	24.50	D	O
	ATOM	6664	N	LYS	195	0.397	-85.999	155.949	1.00	24.56	D	N
	ATOM	6665	CA	LYS	195	1.287	-84.971	156.462	1.00	25.60	D	C
	ATOM	6666	CB	LYS	195	2.513	-85.642	157.085	1.00	26.77	D	C
	ATOM	6667	CG	LYS	195	3.439	-84.704	157.827	1.00	31.05	D	C
	ATOM	6668	CD	LYS	195	4.510	-85.476	158.608	1.00	33.47	D	C
	ATOM	6669	CE	LYS	195	5.494	-86.190	157.686	1.00	34.73	D	C
10	ATOM	6670	NZ	LYS	195	6.494	-87.008	158.448	1.00	37.37	D	N
	ATOM	6671	C	LYS	195	1.715	-83.990	155.349	1.00	24.73	D	C
	ATOM	6672	O	LYS	195	1.796	-82.776	155.569	1.00	23.70	D	O
	ATOM	6673	N	GLY	196	1.967	-84.513	154.152	1.00	22.84	D	N
15	ATOM	6674	CA	GLY	196	2.386	-83.652	153.062	1.00	21.25	D	C
	ATOM	6675	C	GLY	196	1.284	-82.952	152.282	1.00	20.83	D	C
	ATOM	6676	O	GLY	196	1.511	-81.894	151.705	1.00	20.29	D	O
	ATOM	6677	N	ALA	197	0.081	-83.512	152.277	1.00	20.54	D	N
	ATOM	6678	CA	ALA	197	-1.011	-82.932	151.504	1.00	19.62	D	C
20	ATOM	6679	CB	ALA	197	-1.525	-83.983	150.522	1.00	18.07	D	C
	ATOM	6680	C	ALA	197	-2.201	-82.320	152.248	1.00	18.74	D	C
	ATOM	6681	O	ALA	197	-3.011	-81.622	151.634	1.00	17.93	D	O
	ATOM	6682	N	ALA	198	-2.331	-82.589	153.542	1.00	18.19	D	N
	ATOM	6683	CA	ALA	198	-3.474	-82.078	154.311	1.00	17.94	D	C
	ATOM	6684	CB	ALA	198	-3.275	-82.371	155.805	1.00	18.85	D	C
25	ATOM	6685	C	ALA	198	-3.767	-80.588	154.102	1.00	16.59	D	C
	ATOM	6686	O	ALA	198	-4.883	-80.211	153.758	1.00	15.86	D	O
	ATOM	6687	N	VAL	199	-2.770	-79.741	154.320	1.00	16.08	D	N
	ATOM	6688	CA	VAL	199	-2.951	-78.306	154.142	1.00	16.51	D	C
	ATOM	6689	CB	VAL	199	-1.648	-77.545	154.467	1.00	16.75	D	C
30	ATOM	6690	CG1	VAL	199	-1.814	-76.066	154.138	1.00	18.24	D	C
	ATOM	6691	CG2	VAL	199	-1.306	-77.713	155.945	1.00	18.67	D	C
	ATOM	6692	C	VAL	199	-3.395	-77.971	152.709	1.00	16.12	D	C
	ATOM	6693	O	VAL	199	-4.300	-77.156	152.498	1.00	14.02	D	O
	ATOM	6694	N	GLU	200	-2.755	-78.601	151.727	1.00	15.48	D	N
35	ATOM	6695	CA	GLU	200	-3.097	-78.366	150.330	1.00	16.73	D	C
	ATOM	6696	CB	GLU	200	-2.150	-79.157	149.417	1.00	16.50	D	C
	ATOM	6697	CG	GLU	200	-0.768	-78.516	149.252	1.00	17.80	D	C
	ATOM	6698	CD	GLU	200	0.241	-79.419	148.533	1.00	19.22	D	C
	ATOM	6699	OE1	GLU	200	-0.122	-80.054	147.521	1.00	20.12	D	O
40	ATOM	6700	OE2	GLU	200	1.404	-79.481	148.975	1.00	18.83	D	O
	ATOM	6701	C	GLU	200	-4.557	-78.721	150.035	1.00	15.98	D	C
	ATOM	6702	O	GLU	200	-5.285	-77.941	149.402	1.00	15.85	D	O
	ATOM	6703	N	ILE	201	-4.989	-79.890	150.499	1.00	15.63	D	N
	ATOM	6704	CA	ILE	201	-6.364	-80.340	150.293	1.00	15.51	D	C
45	ATOM	6705	CB	ILE	201	-6.575	-81.743	150.927	1.00	15.91	D	C
	ATOM	6706	CG2	ILE	201	-8.058	-82.111	150.932	1.00	15.40	D	C
	ATOM	6707	CG1	ILE	201	-5.766	-82.783	150.129	1.00	18.12	D	C
	ATOM	6708	CD1	ILE	201	-5.472	-84.091	150.870	1.00	15.80	D	C
	ATOM	6709	C	ILE	201	-7.342	-79.327	150.895	1.00	15.21	D	C
50	ATOM	6710	O	ILE	201	-8.321	-78.927	150.251	1.00	14.04	D	O
	ATOM	6711	N	CYS	202	-7.065	-78.892	152.119	1.00	14.29	D	N
	ATOM	6712	CA	CYS	202	-7.934	-77.927	152.776	1.00	15.16	D	C
	ATOM	6713	CB	CYS	202	-7.383	-77.554	154.155	1.00	14.22	D	C
	ATOM	6714	SG	CYS	202	-7.474	-78.932	155.348	1.00	16.23	D	S
55	ATOM	6715	C	CYS	202	-8.124	-76.679	151.931	1.00	14.68	D	C
	ATOM	6716	O	CYS	202	-9.243	-76.190	151.809	1.00	13.66	D	O
	ATOM	6717	N	HIS	203	-7.044	-76.163	151.343	1.00	14.61	D	N
	ATOM	6718	CA	HIS	203	-7.171	-74.974	150.509	1.00	15.81	D	C
	ATOM	6719	CB	HIS	203	-5.797	-74.416	150.140	1.00	15.81	D	C
	ATOM	6720	CG	HIS	203	-5.186	-73.588	151.227	1.00	16.92	D	C

-285-

5	ATOM	6721	CD2	HIS	203	-4.115	-73.810	152.024	1.00	17.06	D	C
	ATOM	6722	ND1	HIS	203	-5.725	-72.389	151.636	1.00	17.22	D	N
	ATOM	6723	CE1	HIS	203	-5.015	-71.905	152.638	1.00	17.87	D	C
	ATOM	6724	NE2	HIS	203	-4.031	-72.749	152.893	1.00	18.68	D	N
	ATOM	6725	C	HIS	203	-7.993	-75.249	149.261	1.00	15.18	D	C
10	ATOM	6726	O	HIS	203	-8.745	-74.395	148.814	1.00	14.74	D	O
	ATOM	6727	N	ILE	204	-7.849	-76.441	148.695	1.00	15.83	D	N
	ATOM	6728	CA	ILE	204	-8.627	-76.797	147.515	1.00	15.89	D	C
	ATOM	6729	CB	ILE	204	-8.230	-78.195	146.994	1.00	16.42	D	C
	ATOM	6730	CG2	ILE	204	-9.213	-78.664	145.904	1.00	15.76	D	C
15	ATOM	6731	CG1	ILE	204	-6.796	-78.148	146.458	1.00	16.43	D	C
	ATOM	6732	CD1	ILE	204	-6.269	-79.496	145.969	1.00	18.76	D	C
	ATOM	6733	C	ILE	204	-10.108	-76.793	147.895	1.00	16.28	D	C
	ATOM	6734	O	ILE	204	-10.943	-76.240	147.175	1.00	15.45	D	O
	ATOM	6735	N	VAL	205	-10.423	-77.393	149.043	1.00	15.70	D	N
20	ATOM	6736	CA	VAL	205	-11.799	-77.474	149.528	1.00	16.11	D	C
	ATOM	6737	CB	VAL	205	-11.895	-78.420	150.759	1.00	16.88	D	C
	ATOM	6738	CG1	VAL	205	-13.274	-78.292	151.427	1.00	16.36	D	C
	ATOM	6739	CG2	VAL	205	-11.661	-79.862	150.315	1.00	16.38	D	C
	ATOM	6740	C	VAL	205	-12.340	-76.103	149.906	1.00	16.68	D	C
25	ATOM	6741	O	VAL	205	-13.452	-75.747	149.545	1.00	16.11	D	O
	ATOM	6742	N	LEU	206	-11.544	-75.330	150.635	1.00	16.97	D	N
	ATOM	6743	CA	LEU	206	-11.962	-74.004	151.057	1.00	18.74	D	C
	ATOM	6744	CB	LEU	206	-10.932	-73.433	152.041	1.00	19.59	D	C
	ATOM	6745	CG	LEU	206	-11.376	-73.183	153.491	1.00	21.97	D	C
30	ATOM	6746	CD1	LEU	206	-12.446	-74.167	153.922	1.00	23.35	D	C
	ATOM	6747	CD2	LEU	206	-10.167	-73.273	154.403	1.00	22.61	D	C
	ATOM	6748	C	LEU	206	-12.178	-73.035	149.886	1.00	18.61	D	C
	ATOM	6749	O	LEU	206	-12.896	-72.045	150.023	1.00	18.78	D	O
	ATOM	6750	N	ASN	207	-11.570	-73.321	148.740	1.00	17.84	D	N
35	ATOM	6751	CA	ASN	207	-11.719	-72.462	147.569	1.00	18.81	D	C
	ATOM	6752	CB	ASN	207	-10.985	-73.050	146.358	1.00	16.45	D	C
	ATOM	6753	CG	ASN	207	-10.986	-72.105	145.167	1.00	17.11	D	C
	ATOM	6754	OD1	ASN	207	-11.660	-72.345	144.162	1.00	13.45	D	O
	ATOM	6755	ND2	ASN	207	-10.235	-71.010	145.283	1.00	15.61	D	N
40	ATOM	6756	C	ASN	207	-13.178	-72.222	147.206	1.00	19.76	D	C
	ATOM	6757	O	ASN	207	-13.527	-71.138	146.727	1.00	19.75	D	O
	ATOM	6758	N	THR	208	-14.037	-73.214	147.442	1.00	20.34	D	N
	ATOM	6759	CA	THR	208	-15.450	-73.050	147.111	1.00	22.21	D	C
	ATOM	6760	CB	THR	208	-16.246	-74.380	147.240	1.00	23.45	D	C
45	ATOM	6761	OG1	THR	208	-16.220	-74.839	148.599	1.00	23.83	D	O
	ATOM	6762	CG2	THR	208	-15.639	-75.453	146.332	1.00	24.88	D	C
	ATOM	6763	C	THR	208	-16.149	-71.972	147.938	1.00	21.89	D	C
	ATOM	6764	O	THR	208	-17.273	-71.599	147.626	1.00	23.81	D	O
	ATOM	6765	N	THR	209	-15.497	-71.465	148.981	1.00	20.43	D	N
50	ATOM	6766	CA	THR	209	-16.098	-70.404	149.799	1.00	19.96	D	C
	ATOM	6767	CB	THR	209	-15.875	-70.626	151.320	1.00	18.96	D	C
	ATOM	6768	OG1	THR	209	-14.496	-70.413	151.632	1.00	17.92	D	O
	ATOM	6769	CG2	THR	209	-16.264	-72.040	151.732	1.00	18.80	D	C
	ATOM	6770	C	THR	209	-15.494	-69.041	149.455	1.00	19.40	D	C
55	ATOM	6771	O	THR	209	-15.903	-68.018	150.008	1.00	19.55	D	O
	ATOM	6772	N	PHE	210	-14.526	-69.030	148.544	1.00	19.55	D	N
	ATOM	6773	CA	PHE	210	-13.846	-67.799	148.151	1.00	20.20	D	C
	ATOM	6774	CB	PHE	210	-12.528	-68.127	147.433	1.00	19.49	D	C
	ATOM	6775	CG	PHE	210	-11.595	-66.951	147.289	1.00	18.07	D	C
	ATOM	6776	CD1	PHE	210	-10.928	-66.432	148.396	1.00	18.57	D	C
	ATOM	6777	CD2	PHE	210	-11.375	-66.367	146.046	1.00	18.17	D	C
	ATOM	6778	CE1	PHE	210	-10.054	-65.350	148.265	1.00	17.81	D	C

-286-

	ATOM	6779	CE2	PHE	210	-10.500	-65.281	145.902	1.00	17.22	D	C
	ATOM	6780	CZ	PHE	210	-9.841	-64.775	147.011	1.00	18.25	D	C
	ATOM	6781	C	PHE	210	-14.722	-66.958	147.240	1.00	21.26	D	C
5.	ATOM	6782	O	PHE	210	-15.199	-67.428	146.212	1.00	20.72	D	O
	ATOM	6783	N	CYS	211	-14.926	-65.708	147.630	1.00	23.14	D	N
	ATOM	6784	CA	CYS	211	-15.736	-64.776	146.862	1.00	25.64	D	C
	ATOM	6785	CB	CYS	211	-16.594	-63.928	147.803	1.00	26.00	D	C
	ATOM	6786	SG	CYS	211	-17.553	-62.630	146.984	1.00	28.41	D	S
10	ATOM	6787	C	CYS	211	-14.812	-63.880	146.044	1.00	27.00	D	C
	ATOM	6788	O	CYS	211	-14.064	-63.070	146.592	1.00	26.49	D	O
	ATOM	6789	N	LEU	212	-14.865	-64.037	144.728	1.00	28.64	D	N
	ATOM	6790	CA	LEU	212	-14.032	-63.250	143.830	1.00	30.45	D	C
	ATOM	6791	CB	LEU	212	-14.267	-63.683	142.383	1.00	30.47	D	C
	ATOM	6792	CG	LEU	212	-13.780	-65.084	142.006	1.00	30.70	D	C
15	ATOM	6793	CD1	LEU	212	-14.109	-65.364	140.550	1.00	31.20	D	C
	ATOM	6794	CD2	LEU	212	-12.285	-65.183	142.237	1.00	30.24	D	C
	ATOM	6795	C	LEU	212	-14.264	-61.748	143.943	1.00	31.68	D	C
	ATOM	6796	O	LEU	212	-13.327	-60.964	143.793	1.00	31.74	D	O
20	ATOM	6797	N	GLN	213	-15.505	-61.349	144.216	1.00	32.60	D	N
	ATOM	6798	CA	GLN	213	-15.844	-59.935	144.315	1.00	33.45	D	C
	ATOM	6799	CB	GLN	213	-17.366	-59.763	144.407	1.00	36.26	D	C
	ATOM	6800	CG	GLN	213	-17.835	-58.346	144.099	1.00	40.79	D	C
	ATOM	6801	CD	GLN	213	-19.349	-58.213	144.055	1.00	43.35	D	C
25	ATOM	6802	OE1	GLN	213	-20.027	-58.316	145.082	1.00	44.82	D	O
	ATOM	6803	NE2	GLN	213	-19.889	-57.984	142.859	1.00	44.19	D	N
	ATOM	6804	C	GLN	213	-15.175	-59.209	145.478	1.00	32.04	D	C
	ATOM	6805	O	GLN	213	-14.750	-58.067	145.331	1.00	31.86	D	O
	ATOM	6806	N	THR	214	-15.076	-59.867	146.629	1.00	30.21	D	N
30	ATOM	6807	CA	THR	214	-14.467	-59.249	147.803	1.00	28.64	D	C
	ATOM	6808	CB	THR	214	-15.435	-59.283	149.002	1.00	28.97	D	C
	ATOM	6809	OG1	THR	214	-15.878	-60.630	149.218	1.00	28.69	D	O
	ATOM	6810	CG2	THR	214	-16.646	-58.390	148.736	1.00	28.63	D	C
	ATOM	6811	C	THR	214	-13.146	-59.870	148.253	1.00	27.89	D	C
35	ATOM	6812	O	THR	214	-12.523	-59.371	149.184	1.00	27.24	D	O
	ATOM	6813	N	GLN	215	-12.719	-60.949	147.600	1.00	27.59	D	N
	ATOM	6814	CA	GLN	215	-11.475	-61.627	147.969	1.00	27.84	D	C
	ATOM	6815	CB	GLN	215	-10.285	-60.671	147.836	1.00	29.73	D	C
	ATOM	6816	CG	GLN	215	-10.102	-60.059	146.458	1.00	32.60	D	C
40	ATOM	6817	CD	GLN	215	-9.768	-61.086	145.407	1.00	34.25	D	C
	ATOM	6818	OE1	GLN	215	-10.590	-61.407	144.550	1.00	36.19	D	O
	ATOM	6819	NE2	GLN	215	-8.555	-61.617	145.471	1.00	35.54	D	N
	ATOM	6820	C	GLN	215	-11.558	-62.121	149.419	1.00	26.63	D	C
	ATOM	6821	O	GLN	215	-10.579	-62.068	150.158	1.00	25.86	D	O
45	ATOM	6822	N	ASN	216	-12.734	-62.600	149.810	1.00	25.65	D	N
	ATOM	6823	CA	ASN	216	-12.985	-63.097	151.160	1.00	25.70	D	C
	ATOM	6824	CB	ASN	216	-14.110	-62.292	151.812	1.00	27.21	D	C
	ATOM	6825	CG	ASN	216	-13.691	-60.904	152.208	1.00	29.76	D	C
	ATOM	6826	OD1	ASN	216	-14.536	-60.054	152.492	1.00	31.19	D	O
50	ATOM	6827	ND2	ASN	216	-12.384	-60.663	152.258	1.00	31.91	D	N
	ATOM	6828	C	ASN	216	-13.435	-64.550	151.133	1.00	24.52	D	C
	ATOM	6829	O	ASN	216	-13.870	-65.051	150.103	1.00	23.28	D	O
	ATOM	6830	N	PHE	217	-13.330	-65.218	152.276	1.00	23.35	D	N
	ATOM	6831	CA	PHE	217	-13.799	-66.591	152.396	1.00	22.98	D	C
55	ATOM	6832	CB	PHE	217	-12.782	-67.476	153.131	1.00	20.37	D	C
	ATOM	6833	CG	PHE	217	-11.514	-67.727	152.352	1.00	19.81	D	C
	ATOM	6834	CD1	PHE	217	-10.458	-66.824	152.396	1.00	19.27	D	C
	ATOM	6835	CD2	PHE	217	-11.388	-68.859	151.556	1.00	19.27	D	C
	ATOM	6836	CE1	PHE	217	-9.291	-67.043	151.655	1.00	19.72	D	C

-287-

5	ATOM	6837	CE2	PHE	217	-10.228	-69.088	150.811	1.00	19.86	D	C
	ATOM	6838	CZ	PHE	217	-9.177	-68.176	150.862	1.00	19.40	D	C
	ATOM	6839	C	PHE	217	-15.094	-66.486	153.211	1.00	23.95	D	C
	ATOM	6840	O	PHE	217	-15.074	-66.063	154.370	1.00	23.31	D	O
	ATOM	6841	N	LEU	218	-16.216	-66.839	152.591	1.00	24.22	D	N
10	ATOM	6842	CA	LEU	218	-17.508	-66.776	153.261	1.00	25.10	D	C
	ATOM	6843	CB	LEU	218	-18.586	-66.298	152.286	1.00	26.14	D	C
	ATOM	6844	CG	LEU	218	-18.260	-64.972	151.583	1.00	27.28	D	C
	ATOM	6845	CD1	LEU	218	-19.386	-64.588	150.624	1.00	26.98	D	C
	ATOM	6846	CD2	LEU	218	-18.041	-63.883	152.640	1.00	27.40	D	C
15	ATOM	6847	C	LEU	218	-17.838	-68.163	153.786	1.00	25.53	D	C
	ATOM	6848	O	LEU	218	-18.116	-69.087	153.019	1.00	25.80	D	O
	ATOM	6849	N	CYS	219	-17.794	-68.306	155.103	1.00	25.26	D	N
	ATOM	6850	CA	CYS	219	-18.055	-69.588	155.733	1.00	25.79	D	C
	ATOM	6851	CB	CYS	219	-16.798	-70.044	156.477	1.00	25.11	D	C
20	ATOM	6852	SG	CYS	219	-15.326	-70.090	155.391	1.00	24.90	D	S
	ATOM	6853	C	CYS	219	-19.249	-69.482	156.674	1.00	25.79	D	C
	ATOM	6854	O	CYS	219	-19.103	-69.165	157.857	1.00	25.32	D	O
	ATOM	6855	N	GLY	220	-20.431	-69.756	156.131	1.00	25.40	D	N
	ATOM	6856	CA	GLY	220	-21.636	-69.660	156.922	1.00	24.69	D	C
25	ATOM	6857	C	GLY	220	-21.761	-68.211	157.341	1.00	24.74	D	C
	ATOM	6858	O	GLY	220	-21.814	-67.325	156.492	1.00	24.53	D	O
	ATOM	6859	N	PRO	221	-21.795	-67.933	158.649	1.00	24.44	D	N
	ATOM	6860	CD	PRO	221	-21.952	-68.897	159.758	1.00	24.16	D	C
	ATOM	6861	CA	PRO	221	-21.912	-66.552	159.119	1.00	24.43	D	C
30	ATOM	6862	CB	PRO	221	-22.545	-66.722	160.495	1.00	25.03	D	C
	ATOM	6863	CG	PRO	221	-21.911	-68.011	160.983	1.00	24.72	D	C
	ATOM	6864	C	PRO	221	-20.573	-65.816	159.192	1.00	24.14	D	C
	ATOM	6865	O	PRO	221	-20.532	-64.601	159.401	1.00	24.82	D	O
	ATOM	6866	N	LEU	222	-19.482	-66.552	159.014	1.00	23.02	D	N
35	ATOM	6867	CA	LEU	222	-18.143	-65.975	159.097	1.00	22.19	D	C
	ATOM	6868	CB	LEU	222	-17.171	-67.006	159.675	1.00	20.44	D	C
	ATOM	6869	CG	LEU	222	-17.611	-67.653	160.991	1.00	19.18	D	C
	ATOM	6870	CD1	LEU	222	-16.513	-68.600	161.478	1.00	18.47	D	C
	ATOM	6871	CD2	LEU	222	-17.900	-66.577	162.031	1.00	17.33	D	C
40	ATOM	6872	C	LEU	222	-17.593	-65.454	157.771	1.00	21.62	D	C
	ATOM	6873	O	LEU	222	-17.955	-65.928	156.697	1.00	21.70	D	O
	ATOM	6874	N	ARG	223	-16.701	-64.480	157.871	1.00	21.04	D	N
	ATOM	6875	CA	ARG	223	-16.072	-63.870	156.709	1.00	21.51	D	C
	ATOM	6876	CB	ARG	223	-16.751	-62.521	156.424	1.00	22.86	D	C
45	ATOM	6877	CG	ARG	223	-16.164	-61.719	155.282	1.00	25.93	D	C
	ATOM	6878	CD	ARG	223	-15.400	-60.495	155.770	1.00	27.48	D	C
	ATOM	6879	NE	ARG	223	-16.221	-59.538	156.520	1.00	28.36	D	N
	ATOM	6880	CZ	ARG	223	-16.287	-59.468	157.850	1.00	29.02	D	C
	ATOM	6881	NH1	ARG	223	-15.587	-60.303	158.613	1.00	28.03	D	N
50	ATOM	6882	NH2	ARG	223	-17.036	-58.536	158.425	1.00	28.61	D	N
	ATOM	6883	C	ARG	223	-14.591	-63.679	157.043	1.00	20.57	D	C
	ATOM	6884	O	ARG	223	-14.249	-62.850	157.889	1.00	20.75	D	O
	ATOM	6885	N	TYR	224	-13.722	-64.466	156.407	1.00	18.81	D	N
	ATOM	6886	CA	TYR	224	-12.278	-64.373	156.640	1.00	17.92	D	C
55	ATOM	6887	CB	TYR	224	-11.630	-65.758	156.654	1.00	17.02	D	C
	ATOM	6888	CG	TYR	224	-12.135	-66.678	157.744	1.00	17.15	D	C
	ATOM	6889	CD1	TYR	224	-13.245	-67.502	157.530	1.00	17.59	D	C
	ATOM	6890	CE1	TYR	224	-13.707	-68.357	158.524	1.00	17.94	D	C
	ATOM	6891	CD2	TYR	224	-11.503	-66.732	158.981	1.00	15.66	D	C
	ATOM	6892	CE2	TYR	224	-11.957	-67.587	159.985	1.00	16.21	D	C
	ATOM	6893	CZ	TYR	224	-13.059	-68.397	159.749	1.00	16.87	D	C
	ATOM	6894	OH	TYR	224	-13.512	-69.256	160.725	1.00	15.77	D	O

-288-

5	ATOM	6895	C	TYR	224	-11.609	-63.534	155.557	1.00	17.55	D	C
	ATOM	6896	O	TYR	224	-11.878	-63.721	154.378	1.00	16.13	D	O
	ATOM	6897	N	THR	225	-10.718	-62.638	155.972	1.00	16.25	D	N
	ATOM	6898	CA	THR	225	-10.022	-61.751	155.049	1.00	16.87	D	C
	ATOM	6899	CB	THR	225	-10.325	-60.266	155.380	1.00	17.79	D	C
10	ATOM	6900	OG1	THR	225	-9.834	-59.964	156.693	1.00	17.11	D	O
	ATOM	6901	CG2	THR	225	-11.827	-59.993	155.348	1.00	18.41	D	C
	ATOM	6902	C	THR	225	-8.505	-61.926	155.098	1.00	16.77	D	C
	ATOM	6903	O	THR	225	-7.957	-62.593	155.986	1.00	15.99	D	O
	ATOM	6904	N	ILE	226	-7.825	-61.287	154.156	1.00	16.23	D	N
15	ATOM	6905	CA	ILE	226	-6.376	-61.354	154.099	1.00	16.57	D	C
	ATOM	6906	CB	ILE	226	-5.859	-60.731	152.769	1.00	17.02	D	C
	ATOM	6907	CG2	ILE	226	-6.028	-59.202	152.796	1.00	15.14	D	C
	ATOM	6908	CG1	ILE	226	-4.404	-61.149	152.527	1.00	16.61	D	C
	ATOM	6909	CD1	ILE	226	-3.850	-60.691	151.185	1.00	14.79	D	C
20	ATOM	6910	C	ILE	226	-5.769	-60.642	155.327	1.00	17.24	D	C
	ATOM	6911	O	ILE	226	-4.649	-60.956	155.751	1.00	16.91	D	O
	ATOM	6912	N	GLU	227	-6.512	-59.705	155.919	1.00	16.07	D	N
	ATOM	6913	CA	GLU	227	-6.012	-59.006	157.103	1.00	16.95	D	C
	ATOM	6914	CB	GLU	227	-6.915	-57.820	157.495	1.00	16.63	D	C
25	ATOM	6915	CG	GLU	227	-6.820	-56.578	156.571	1.00	16.07	D	C
	ATOM	6916	CD	GLU	227	-7.416	-56.810	155.195	1.00	16.66	D	C
	ATOM	6917	OE1	GLU	227	-8.484	-57.443	155.117	1.00	16.07	D	O
	ATOM	6918	OE2	GLU	227	-6.833	-56.350	154.187	1.00	17.97	D	O
	ATOM	6919	C	GLU	227	-5.918	-59.980	158.280	1.00	16.47	D	C
30	ATOM	6920	O	GLU	227	-5.073	-59.817	159.159	1.00	16.40	D	O
	ATOM	6921	N	ASP	228	-6.782	-60.989	158.309	1.00	15.66	D	N
	ATOM	6922	CA	ASP	228	-6.716	-61.963	159.393	1.00	16.51	D	C
	ATOM	6923	CB	ASP	228	-7.881	-62.953	159.311	1.00	15.72	D	C
	ATOM	6924	CG	ASP	228	-9.220	-62.286	159.555	1.00	16.63	D	C
35	ATOM	6925	OD1	ASP	228	-9.328	-61.514	160.540	1.00	16.26	D	O
	ATOM	6926	OD2	ASP	228	-10.160	-62.531	158.768	1.00	16.57	D	O
	ATOM	6927	C	ASP	228	-5.381	-62.709	159.361	1.00	15.84	D	C
	ATOM	6928	O	ASP	228	-4.791	-62.970	160.406	1.00	17.26	D	O
	ATOM	6929	N	GLY	229	-4.905	-63.047	158.164	1.00	15.54	D	N
40	ATOM	6930	CA	GLY	229	-3.629	-63.735	158.053	1.00	14.97	D	C
	ATOM	6931	C	GLY	229	-2.474	-62.803	158.385	1.00	15.19	D	C
	ATOM	6932	O	GLY	229	-1.484	-63.204	159.010	1.00	14.72	D	O
	ATOM	6933	N	ALA	230	-2.600	-61.544	157.973	1.00	13.93	D	N
	ATOM	6934	CA	ALA	230	-1.557	-60.564	158.233	1.00	14.50	D	C
45	ATOM	6935	CB	ALA	230	-1.844	-59.279	157.456	1.00	14.94	D	C
	ATOM	6936	C	ALA	230	-1.445	-60.268	159.732	1.00	14.36	D	C
	ATOM	6937	O	ALA	230	-0.341	-60.150	160.263	1.00	12.75	D	O
	ATOM	6938	N	ARG	231	-2.588	-60.164	160.410	1.00	14.18	D	N
	ATOM	6939	CA	ARG	231	-2.596	-59.877	161.840	1.00	15.32	D	C
50	ATOM	6940	CB	ARG	231	-4.014	-59.504	162.324	1.00	15.52	D	C
	ATOM	6941	CG	ARG	231	-4.594	-58.198	161.761	1.00	18.02	D	C
	ATOM	6942	CD	ARG	231	-3.828	-56.948	162.224	1.00	19.48	D	C
	ATOM	6943	NE	ARG	231	-3.939	-56.687	163.665	1.00	21.35	D	N
	ATOM	6944	CZ	ARG	231	-4.921	-55.994	164.246	1.00	22.41	D	C
55	ATOM	6945	NH1	ARG	231	-5.906	-55.470	163.527	1.00	20.52	D	N
	ATOM	6946	NH2	ARG	231	-4.911	-55.809	165.559	1.00	23.57	D	N
	ATOM	6947	C	ARG	231	-2.044	-61.026	162.698	1.00	14.73	D	C
	ATOM	6948	O	ARG	231	-1.608	-60.781	163.805	1.00	14.28	D	O
	ATOM	6949	N	VAL	232	-2.071	-62.271	162.220	1.00	14.81	D	N
	ATOM	6950	CA	VAL	232	-1.516	-63.349	163.038	1.00	15.74	D	C
	ATOM	6951	CB	VAL	232	-2.273	-64.700	162.869	1.00	16.44	D	C
	ATOM	6952	CG1	VAL	232	-3.736	-64.514	163.233	1.00	17.47	D	C

-289-

	ATOM	6953	CG2	VAL	232	-2.115	-65.247	161.447	1.00	16.56	D	C
	ATOM	6954	C	VAL	232	-0.028	-63.552	162.744	1.00	15.66	D	C
	ATOM	6955	O	VAL	232	0.607	-64.442	163.302	1.00	14.93	D	O
5	ATOM	6956	N	GLY	233	0.529	-62.719	161.868	1.00	15.13	D	N
	ATOM	6957	CA	GLY	233	1.946	-62.818	161.586	1.00	15.93	D	C
	ATOM	6958	C	GLY	233	2.433	-63.251	160.218	1.00	16.55	D	C
	ATOM	6959	O	GLY	233	3.630	-63.157	159.961	1.00	16.84	D	O
	ATOM	6960	N	PHE	234	1.555	-63.741	159.347	1.00	16.39	D	N
10	ATOM	6961	CA	PHE	234	2.008	-64.144	158.017	1.00	17.11	D	C
	ATOM	6962	CB	PHE	234	0.882	-64.815	157.226	1.00	16.36	D	C
	ATOM	6963	CG	PHE	234	0.537	-66.194	157.703	1.00	16.05	D	C
	ATOM	6964	CD1	PHE	234	-0.647	-66.429	158.386	1.00	14.44	D	C
	ATOM	6965	CD2	PHE	234	1.382	-67.273	157.420	1.00	15.78	D	C
15	ATOM	6966	CE1	PHE	234	-0.998	-67.724	158.779	1.00	16.61	D	C
	ATOM	6967	CE2	PHE	234	1.043	-68.570	157.807	1.00	15.23	D	C
	ATOM	6968	CZ	PHE	234	-0.150	-68.799	158.486	1.00	15.89	D	C
	ATOM	6969	C	PHE	234	2.485	-62.930	157.234	1.00	18.16	D	C
	ATOM	6970	O	PHE	234	1.902	-61.844	157.340	1.00	18.39	D	O
20	ATOM	6971	N	GLN	235	3.547	-63.112	156.451	1.00	19.12	D	N
	ATOM	6972	CA	GLN	235	4.080	-62.032	155.624	1.00	19.59	D	C
	ATOM	6973	CB	GLN	235	5.445	-62.396	155.052	1.00	21.47	D	C
	ATOM	6974	CG	GLN	235	6.546	-62.520	156.080	1.00	25.04	D	C
	ATOM	6975	CD	GLN	235	7.882	-62.810	155.433	1.00	27.60	D	C
25	ATOM	6976	OE1	GLN	235	8.009	-63.749	154.643	1.00	28.65	D	O
	ATOM	6977	NE2	GLN	235	8.890	-62.006	155.760	1.00	28.31	D	N
	ATOM	6978	C	GLN	235	3.117	-61.786	154.476	1.00	19.54	D	C
	ATOM	6979	O	GLN	235	2.544	-62.721	153.920	1.00	18.79	D	O
	ATOM	6980	N	VAL	236	2.954	-60.519	154.119	1.00	19.32	D	N
30	ATOM	6981	CA	VAL	236	2.046	-60.123	153.053	1.00	19.50	D	C
	ATOM	6982	CB	VAL	236	2.089	-58.590	152.866	1.00	19.33	D	C
	ATOM	6983	CG1	VAL	236	1.275	-58.181	151.660	1.00	18.53	D	C
	ATOM	6984	CG2	VAL	236	1.577	-57.913	154.126	1.00	18.96	D	C
	ATOM	6985	C	VAL	236	2.294	-60.806	151.708	1.00	19.71	D	C
35	ATOM	6986	O	VAL	236	1.352	-61.243	151.058	1.00	19.46	D	O
	ATOM	6987	N	GLU	237	3.551	-60.888	151.287	1.00	20.19	D	N
	ATOM	6988	CA	GLU	237	3.892	-61.523	150.014	1.00	21.32	D	C
	ATOM	6989	CB	GLU	237	5.407	-61.463	149.802	1.00	23.35	D	C
	ATOM	6990	CG	GLU	237	5.888	-62.029	148.485	1.00	27.69	D	C
40	ATOM	6991	CD	GLU	237	7.288	-61.544	148.135	1.00	31.29	D	C
	ATOM	6992	OE1	GLU	237	7.435	-60.350	147.778	1.00	33.68	D	O
	ATOM	6993	OE2	GLU	237	8.239	-62.346	148.229	1.00	32.41	D	O
	ATOM	6994	C	GLU	237	3.396	-62.975	149.960	1.00	20.15	D	C
	ATOM	6995	O	GLU	237	2.873	-63.428	148.942	1.00	19.45	D	O
45	ATOM	6996	N	PHE	238	3.567	-63.697	151.061	1.00	18.94	D	N
	ATOM	6997	CA	PHE	238	3.110	-65.076	151.152	1.00	18.95	D	C
	ATOM	6998	CB	PHE	238	3.507	-65.656	152.511	1.00	18.87	D	C
	ATOM	6999	CG	PHE	238	2.793	-66.922	152.862	1.00	18.24	D	C
	ATOM	7000	CD1	PHE	238	3.121	-68.122	152.239	1.00	18.39	D	C
50	ATOM	7001	CD2	PHE	238	1.769	-66.911	153.797	1.00	18.85	D	C
	ATOM	7002	CE1	PHE	238	2.433	-69.297	152.545	1.00	18.05	D	C
	ATOM	7003	CE2	PHE	238	1.075	-68.079	154.109	1.00	19.77	D	C
	ATOM	7004	CZ	PHE	238	1.410	-69.274	153.480	1.00	18.89	D	C
	ATOM	7005	C	PHE	238	1.586	-65.064	150.998	1.00	19.39	D	C
55	ATOM	7006	O	PHE	238	1.018	-65.854	150.239	1.00	18.49	D	O
	ATOM	7007	N	LEU	239	0.940	-64.143	151.713	1.00	18.74	D	N
	ATOM	7008	CA	LEU	239	-0.510	-63.986	151.675	1.00	19.82	D	C
	ATOM	7009	CB	LEU	239	-0.942	-62.852	152.611	1.00	18.63	D	C
	ATOM	7010	CG	LEU	239	-1.538	-63.153	153.992	1.00	19.49	D	C

-290-

	ATOM	7011	CD1	LEU	239	-1.136	-64.510	154.487	1.00	16.15	D	C
	ATOM	7012	CD2	LEU	239	-1.118	-62.049	154.954	1.00	16.47	D	C
	ATOM	7013	C	LEU	239	-1.012	-63.697	150.268	1.00	20.21	D	C
5	ATOM	7014	O	LEU	239	-1.976	-64.315	149.819	1.00	19.21	D	O
	ATOM	7015	N	GLU	240	-0.370	-62.755	149.578	1.00	20.94	D	N
	ATOM	7016	CA	GLU	240	-0.776	-62.413	148.216	1.00	22.99	D	C
	ATOM	7017	CB	GLU	240	0.069	-61.255	147.664	1.00	25.70	D	C
	ATOM	7018	CG	GLU	240	-0.191	-59.897	148.330	1.00	28.57	D	C
10	ATOM	7019	CD	GLU	240	-1.584	-59.334	148.036	1.00	32.06	D	C
	ATOM	7020	OE1	GLU	240	-2.437	-60.068	147.492	1.00	33.41	D	O
	ATOM	7021	OE2	GLU	240	-1.834	-58.151	148.358	1.00	34.50	D	O
	ATOM	7022	C	GLU	240	-0.649	-63.633	147.304	1.00	22.86	D	C
	ATOM	7023	O	GLU	240	-1.510	-63.874	146.469	1.00	22.97	D	O
15	ATOM	7024	N	LEU	241	0.424	-64.400	147.462	1.00	22.57	D	N
	ATOM	7025	CA	LEU	241	0.618	-65.603	146.655	1.00	23.67	D	C
	ATOM	7026	CB	LEU	241	1.948	-66.270	147.035	1.00	25.60	D	C
	ATOM	7027	CG	LEU	241	2.655	-67.315	146.151	1.00	28.83	D	C
	ATOM	7028	CD1	LEU	241	1.856	-68.588	146.108	1.00	30.65	D	C
20	ATOM	7029	CD2	LEU	241	2.858	-66.775	144.748	1.00	29.93	D	C
	ATOM	7030	C	LEU	241	-0.567	-66.551	146.931	1.00	22.49	D	C
	ATOM	7031	O	LEU	241	-1.150	-67.113	146.013	1.00	21.13	D	O
	ATOM	7032	N	LEU	242	-0.937	-66.692	148.201	1.00	21.14	D	N
	ATOM	7033	CA	LEU	242	-2.041	-67.559	148.588	1.00	20.53	D	C
25	ATOM	7034	CB	LEU	242	-2.129	-67.648	150.114	1.00	21.39	D	C
	ATOM	7035	CG	LEU	242	-3.315	-68.423	150.701	1.00	22.85	D	C
	ATOM	7036	CD1	LEU	242	-3.410	-69.821	150.090	1.00	22.86	D	C
	ATOM	7037	CD2	LEU	242	-3.144	-68.507	152.211	1.00	22.33	D	C
	ATOM	7038	C	LEU	242	-3.383	-67.106	148.017	1.00	20.15	D	C
30	ATOM	7039	O	LEU	242	-4.119	-67.913	147.438	1.00	19.21	D	O
	ATOM	7040	N	PHE	243	-3.699	-65.819	148.160	1.00	19.18	D	N
	ATOM	7041	CA	PHE	243	-4.967	-65.307	147.646	1.00	19.02	D	C
	ATOM	7042	CB	PHE	243	-5.285	-63.928	148.242	1.00	17.31	D	C
	ATOM	7043	CG	PHE	243	-5.842	-63.993	149.650	1.00	16.71	D	C
35	ATOM	7044	CD1	PHE	243	-5.054	-64.440	150.713	1.00	15.59	D	C
	ATOM	7045	CD2	PHE	243	-7.167	-63.645	149.905	1.00	16.40	D	C
	ATOM	7046	CE1	PHE	243	-5.573	-64.542	152.009	1.00	15.90	D	C
	ATOM	7047	CE2	PHE	243	-7.703	-63.744	151.204	1.00	16.02	D	C
	ATOM	7048	CZ	PHE	243	-6.901	-64.194	152.254	1.00	15.02	D	C
40	ATOM	7049	C	PHE	243	-5.017	-65.269	146.117	1.00	19.44	D	C
	ATOM	7050	O	PHE	243	-6.094	-65.356	145.533	1.00	18.99	D	O
	ATOM	7051	N	HIS	244	-3.858	-65.144	145.474	1.00	19.69	D	N
	ATOM	7052	CA	HIS	244	-3.804	-65.152	144.016	1.00	20.80	D	C
	ATOM	7053	CB	HIS	244	-2.404	-64.783	143.505	1.00	22.74	D	C
45	ATOM	7054	CG	HIS	244	-2.235	-64.959	142.025	1.00	26.38	D	C
	ATOM	7055	CD2	HIS	244	-2.396	-64.088	140.999	1.00	27.16	D	C
	ATOM	7056	ND1	HIS	244	-1.905	-66.170	141.448	1.00	27.90	D	N
	ATOM	7057	CE1	HIS	244	-1.873	-66.036	140.134	1.00	27.13	D	C
	ATOM	7058	NE2	HIS	244	-2.167	-64.783	139.836	1.00	27.37	D	N
50	ATOM	7059	C	HIS	244	-4.149	-66.570	143.591	1.00	19.50	D	C
	ATOM	7060	O	HIS	244	-4.868	-66.775	142.621	1.00	18.50	D	O
	ATOM	7061	N	PHE	245	-3.627	-67.550	144.326	1.00	18.62	D	N
	ATOM	7062	CA	PHE	245	-3.917	-68.946	144.036	1.00	17.80	D	C
	ATOM	7063	CB	PHE	245	-3.244	-69.871	145.055	1.00	17.14	D	C
	ATOM	7064	CG	PHE	245	-3.817	-71.265	145.069	1.00	16.75	D	C
55	ATOM	7065	CD1	PHE	245	-3.442	-72.197	144.105	1.00	16.57	D	C
	ATOM	7066	CD2	PHE	245	-4.784	-71.624	146.007	1.00	16.20	D	C
	ATOM	7067	CE1	PHE	245	-4.024	-73.467	144.068	1.00	16.23	D	C
	ATOM	7068	CE2	PHE	245	-5.372	-72.884	145.984	1.00	16.41	D	C

-291-

	ATOM	7069	CZ	PHE	245	-4.992	-73.812	145.009	1.00	15.98	D	C
	ATOM	7070	C	PHE	245	-5.430	-69.170	144.100	1.00	17.44	D	C
	ATOM	7071	O	PHE	245	-6.005	-69.787	143.212	1.00	17.41	D	O
5	ATOM	7072	N	HIS	246	-6.068	-68.669	145.154	1.00	16.27	D	N
	ATOM	7073	CA	HIS	246	-7.505	-68.853	145.316	1.00	16.76	D	C
	ATOM	7074	CB	HIS	246	-7.939	-68.409	146.717	1.00	14.87	D	C
	ATOM	7075	CG	HIS	246	-7.740	-69.466	147.761	1.00	15.84	D	C
	ATOM	7076	CD2	HIS	246	-6.779	-69.620	148.702	1.00	14.94	D	C
10	ATOM	7077	ND1	HIS	246	-8.554	-70.574	147.862	1.00	13.95	D	N
	ATOM	7078	CE1	HIS	246	-8.102	-71.366	148.816	1.00	14.24	D	C
	ATOM	7079	NE2	HIS	246	-7.026	-70.810	149.342	1.00	15.38	D	N
	ATOM	7080	C	HIS	246	-8.334	-68.158	144.242	1.00	16.72	D	C
	ATOM	7081	O	HIS	246	-9.260	-68.750	143.694	1.00	16.62	D	O
15	ATOM	7082	N	GLY	247	-7.999	-66.910	143.940	1.00	16.82	D	N
	ATOM	7083	CA	GLY	247	-8.724	-66.196	142.907	1.00	18.06	D	C
	ATOM	7084	C	GLY	247	-8.606	-66.903	141.569	1.00	18.01	D	C
	ATOM	7085	O	GLY	247	-9.592	-67.087	140.867	1.00	18.60	D	O
	ATOM	7086	N	THR	248	-7.397	-67.324	141.222	1.00	18.13	D	N
20	ATOM	7087	CA	THR	248	-7.162	-68.007	139.953	1.00	18.70	D	C
	ATOM	7088	CB	THR	248	-5.666	-68.298	139.763	1.00	18.46	D	C
	ATOM	7089	OG1	THR	248	-4.933	-67.084	139.926	1.00	19.05	D	O
	ATOM	7090	CG2	THR	248	-5.389	-68.857	138.368	1.00	18.69	D	C
	ATOM	7091	C	THR	248	-7.937	-69.321	139.878	1.00	18.91	D	C
	ATOM	7092	O	THR	248	-8.565	-69.621	138.872	1.00	18.39	D	O
25	ATOM	7093	N	LEU	249	-7.882	-70.110	140.943	1.00	19.20	D	N
	ATOM	7094	CA	LEU	249	-8.593	-71.378	140.969	1.00	20.23	D	C
	ATOM	7095	CB	LEU	249	-8.260	-72.134	142.259	1.00	19.48	D	C
	ATOM	7096	CG	LEU	249	-8.868	-73.523	142.443	1.00	20.29	D	C
	ATOM	7097	CD1	LEU	249	-8.557	-74.390	141.232	1.00	20.40	D	C
30	ATOM	7098	CD2	LEU	249	-8.324	-74.150	143.713	1.00	18.44	D	C
	ATOM	7099	C	LEU	249	-10.104	-71.145	140.867	1.00	20.65	D	C
	ATOM	7100	O	LEU	249	-10.795	-71.821	140.109	1.00	19.63	D	O
	ATOM	7101	N	ARG	250	-10.607	-70.173	141.621	1.00	21.15	D	N
	ATOM	7102	CA	ARG	250	-12.032	-69.862	141.626	1.00	23.18	D	C
35	ATOM	7103	CB	ARG	250	-12.328	-68.773	142.662	1.00	24.41	D	C
	ATOM	7104	CG	ARG	250	-13.164	-69.241	143.835	1.00	27.96	D	C
	ATOM	7105	CD	ARG	250	-14.536	-69.704	143.403	1.00	27.83	D	C
	ATOM	7106	NE	ARG	250	-15.495	-69.580	144.495	1.00	29.89	D	N
	ATOM	7107	CZ	ARG	250	-16.814	-69.673	144.354	1.00	32.93	D	C
40	ATOM	7108	NH1	ARG	250	-17.603	-69.535	145.412	1.00	35.07	D	N
	ATOM	7109	NH2	ARG	250	-17.350	-69.902	143.159	1.00	33.97	D	N
	ATOM	7110	C	ARG	250	-12.614	-69.424	140.284	1.00	23.27	D	C
	ATOM	7111	O	ARG	250	-13.755	-69.749	139.972	1.00	21.85	D	O
	ATOM	7112	N	LYS	251	-11.842	-68.674	139.504	1.00	24.10	D	N
45	ATOM	7113	CA	LYS	251	-12.322	-68.194	138.211	1.00	25.70	D	C
	ATOM	7114	CB	LYS	251	-11.364	-67.141	137.640	1.00	26.54	D	C
	ATOM	7115	CG	LYS	251	-11.350	-65.836	138.421	1.00	27.85	D	C
	ATOM	7116	CD	LYS	251	-10.374	-64.842	137.821	1.00	30.19	D	C
	ATOM	7117	CE	LYS	251	-10.214	-63.616	138.716	1.00	31.63	D	C
50	ATOM	7118	NZ	LYS	251	-9.159	-62.675	138.208	1.00	34.50	D	N
	ATOM	7119	C	LYS	251	-12.523	-69.307	137.190	1.00	26.18	D	C
	ATOM	7120	O	LYS	251	-13.209	-69.112	136.192	1.00	26.51	D	O
	ATOM	7121	N	LEU	252	-11.928	-70.471	137.431	1.00	26.18	D	N
	ATOM	7122	CA	LEU	252	-12.076	-71.588	136.509	1.00	26.53	D	C
55	ATOM	7123	CB	LEU	252	-10.973	-72.617	136.745	1.00	24.32	D	C
	ATOM	7124	CG	LEU	252	-9.535	-72.157	136.495	1.00	23.79	D	C
	ATOM	7125	CD1	LEU	252	-8.583	-73.310	136.786	1.00	21.82	D	C
	ATOM	7126	CD2	LEU	252	-9.378	-71.681	135.054	1.00	22.08	D	C

-292-

	ATOM	7127	C	LEU	252	-13.446	-72.259	136.628	1.00	27.56	D	C
	ATOM	7128	O	LEU	252	-13.794	-73.108	135.812	1.00	28.31	D	O
	ATOM	7129	N	GLN	253	-14.222	-71.868	137.636	1.00	28.57	D	N
5	ATOM	7130	CA	GLN	253	-15.556	-72.421	137.863	1.00	29.80	D	C
	ATOM	7131	CB	GLN	253	-16.554	-71.824	136.862	1.00	31.77	D	C
	ATOM	7132	CG	GLN	253	-16.555	-70.298	136.817	1.00	35.28	D	C
	ATOM	7133	CD	GLN	253	-17.738	-69.711	136.048	1.00	38.18	D	C
	ATOM	7134	OE1	GLN	253	-17.657	-68.597	135.524	1.00	39.03	D	O
10	ATOM	7135	NE2	GLN	253	-18.847	-70.451	135.992	1.00	39.86	D	N
	ATOM	7136	C	GLN	253	-15.576	-73.942	137.752	1.00	29.42	D	C
	ATOM	7137	O	GLN	253	-16.292	-74.502	136.923	1.00	29.12	D	O
	ATOM	7138	N	LEU	254	-14.792	-74.609	138.593	1.00	28.93	D	N
	ATOM	7139	CA	LEU	254	-14.726	-76.065	138.573	1.00	28.81	D	C
15	ATOM	7140	CB	LEU	254	-13.545	-76.572	139.408	1.00	26.92	D	C
	ATOM	7141	CG	LEU	254	-12.129	-76.144	139.015	1.00	26.12	D	C
	ATOM	7142	CD1	LEU	254	-11.123	-76.798	139.947	1.00	23.47	D	C
	ATOM	7143	CD2	LEU	254	-11.865	-76.530	137.571	1.00	25.72	D	C
	ATOM	7144	C	LEU	254	-15.996	-76.687	139.118	1.00	29.64	D	C
20	ATOM	7145	O	LEU	254	-16.728	-76.068	139.891	1.00	29.37	D	O
	ATOM	7146	N	GLN	255	-16.239	-77.926	138.710	1.00	30.18	D	N
	ATOM	7147	CA	GLN	255	-17.392	-78.681	139.164	1.00	31.73	D	C
	ATOM	7148	CB	GLN	255	-17.980	-79.489	138.003	1.00	34.30	D	C
	ATOM	7149	CG	GLN	255	-17.735	-78.843	136.643	1.00	38.01	D	C
25	ATOM	7150	CD	GLN	255	-18.767	-79.210	135.602	1.00	40.76	D	C
	ATOM	7151	OE1	GLN	255	-19.198	-80.360	135.511	1.00	42.15	D	O
	ATOM	7152	NE2	GLN	255	-19.157	-78.230	134.789	1.00	42.18	D	N
	ATOM	7153	C	GLN	255	-16.843	-79.606	140.251	1.00	31.09	D	C
	ATOM	7154	O	GLN	255	-15.639	-79.876	140.292	1.00	29.84	D	O
30	ATOM	7155	N	GLU	256	-17.713	-80.091	141.127	1.00	30.54	D	N
	ATOM	7156	CA	GLU	256	-17.273	-80.951	142.219	1.00	30.46	D	C
	ATOM	7157	CB	GLU	256	-18.477	-81.572	142.920	1.00	32.16	D	C
	ATOM	7158	CG	GLU	256	-19.336	-80.553	143.620	1.00	34.89	D	C
	ATOM	7159	CD	GLU	256	-20.223	-81.178	144.663	1.00	35.98	D	C
35	ATOM	7160	OE1	GLU	256	-20.946	-82.138	144.320	1.00	36.28	D	O
	ATOM	7161	OE2	GLU	256	-20.194	-80.707	145.820	1.00	36.73	D	O
	ATOM	7162	C	GLU	256	-16.270	-82.041	141.861	1.00	29.44	D	C
	ATOM	7163	O	GLU	256	-15.216	-82.139	142.486	1.00	29.52	D	O
	ATOM	7164	N	PRO	257	-16.578	-82.882	140.862	1.00	28.35	D	N
40	ATOM	7165	CD	PRO	257	-17.795	-83.008	140.045	1.00	29.24	D	C
	ATOM	7166	CA	PRO	257	-15.605	-83.927	140.526	1.00	27.52	D	C
	ATOM	7167	CB	PRO	257	-16.260	-84.659	139.347	1.00	27.78	D	C
	ATOM	7168	CG	PRO	257	-17.266	-83.672	138.815	1.00	29.42	D	C
	ATOM	7169	C	PRO	257	-14.197	-83.416	140.215	1.00	25.67	D	C
45	ATOM	7170	O	PRO	257	-13.212	-84.074	140.539	1.00	24.99	D	O
	ATOM	7171	N	GLU	258	-14.098	-82.247	139.590	1.00	24.23	D	N
	ATOM	7172	CA	GLU	258	-12.795	-81.671	139.273	1.00	22.93	D	C
	ATOM	7173	CB	GLU	258	-12.969	-80.476	138.329	1.00	21.97	D	C
	ATOM	7174	CG	GLU	258	-13.493	-80.901	136.971	1.00	23.09	D	C
50	ATOM	7175	CD	GLU	258	-13.973	-79.749	136.109	1.00	22.64	D	C
	ATOM	7176	OE1	GLU	258	-14.538	-78.778	136.653	1.00	22.76	D	O
	ATOM	7177	OE2	GLU	258	-13.808	-79.834	134.876	1.00	22.39	D	O
	ATOM	7178	C	GLU	258	-12.080	-81.259	140.568	1.00	22.29	D	C
	ATOM	7179	O	GLU	258	-10.888	-81.519	140.733	1.00	21.58	D	O
55	ATOM	7180	N	TYR	259	-12.809	-80.625	141.484	1.00	20.81	D	N
	ATOM	7181	CA	TYR	259	-12.227	-80.219	142.762	1.00	20.66	D	C
	ATOM	7182	CB	TYR	259	-13.257	-79.486	143.635	1.00	19.41	D	C
	ATOM	7183	CG	TYR	259	-13.282	-77.985	143.490	1.00	18.07	D	C
	ATOM	7184	CD1	TYR	259	-12.170	-77.210	143.825	1.00	18.03	D	C

-293-

5	ATOM	7185	CE1	TYR	259	-12.205	-75.819	143.728	1.00	16.82	D	C
	ATOM	7186	CD2	TYR	259	-14.429	-77.334	143.047	1.00	17.04	D	C
	ATOM	7187	CE2	TYR	259	-14.478	-75.954	142.940	1.00	16.86	D	C
	ATOM	7188	CZ	TYR	259	-13.363	-75.200	143.285	1.00	17.78	D	C
	ATOM	7189	OH	TYR	259	-13.426	-73.832	143.199	1.00	16.55	D	O
10	ATOM	7190	C	TYR	259	-11.740	-81.442	143.525	1.00	20.57	D	C
	ATOM	7191	O	TYR	259	-10.625	-81.456	144.047	1.00	19.89	D	O
	ATOM	7192	N	VAL	260	-12.568	-82.481	143.586	1.00	20.84	D	N
	ATOM	7193	CA	VAL	260	-12.169	-83.663	144.333	1.00	21.82	D	C
	ATOM	7194	CB	VAL	260	-13.386	-84.618	144.586	1.00	23.38	D	C
15	ATOM	7195	CG1	VAL	260	-13.761	-85.380	143.328	1.00	23.89	D	C
	ATOM	7196	CG2	VAL	260	-13.064	-85.566	145.719	1.00	24.50	D	C
	ATOM	7197	C	VAL	260	-11.004	-84.395	143.679	1.00	21.20	D	C
	ATOM	7198	O	VAL	260	-10.147	-84.937	144.373	1.00	21.64	D	O
	ATOM	7199	N	LEU	261	-10.949	-84.398	142.353	1.00	20.69	D	N
20	ATOM	7200	CA	LEU	261	-9.841	-85.056	141.656	1.00	21.07	D	C
	ATOM	7201	CB	LEU	261	-10.132	-85.156	140.158	1.00	21.76	D	C
	ATOM	7202	CG	LEU	261	-11.172	-86.227	139.803	1.00	21.71	D	C
	ATOM	7203	CD1	LEU	261	-11.584	-86.102	138.346	1.00	21.95	D	C
	ATOM	7204	CD2	LEU	261	-10.584	-87.611	140.090	1.00	20.53	D	C
25	ATOM	7205	C	LEU	261	-8.553	-84.280	141.897	1.00	21.22	D	C
	ATOM	7206	O	LEU	261	-7.476	-84.860	141.996	1.00	21.66	D	O
	ATOM	7207	N	LEU	262	-8.671	-82.960	141.999	1.00	21.22	D	N
	ATOM	7208	CA	LEU	262	-7.517	-82.110	142.266	1.00	21.43	D	C
	ATOM	7209	CB	LEU	262	-7.946	-80.647	142.212	1.00	23.16	D	C
30	ATOM	7210	CG	LEU	262	-6.936	-79.598	141.743	1.00	25.15	D	C
	ATOM	7211	CD1	LEU	262	-6.356	-79.997	140.390	1.00	24.87	D	C
	ATOM	7212	CD2	LEU	262	-7.649	-78.248	141.647	1.00	26.33	D	C
	ATOM	7213	C	LEU	262	-6.989	-82.460	143.663	1.00	21.12	D	C
	ATOM	7214	O	LEU	262	-5.780	-82.568	143.877	1.00	20.89	D	O
35	ATOM	7215	N	ALA	263	-7.909	-82.643	144.608	1.00	19.39	D	N
	ATOM	7216	CA	ALA	263	-7.546	-83.001	145.972	1.00	19.66	D	C
	ATOM	7217	CB	ALA	263	-8.797	-83.038	146.865	1.00	18.64	D	C
	ATOM	7218	C	ALA	263	-6.845	-84.357	145.989	1.00	19.63	D	C
	ATOM	7219	O	ALA	263	-5.847	-84.534	146.686	1.00	19.49	D	O
40	ATOM	7220	N	ALA	264	-7.366	-85.310	145.216	1.00	19.23	D	N
	ATOM	7221	CA	ALA	264	-6.773	-86.639	145.136	1.00	19.14	D	C
	ATOM	7222	CB	ALA	264	-7.670	-87.563	144.300	1.00	18.99	D	C
	ATOM	7223	C	ALA	264	-5.366	-86.566	144.518	1.00	19.43	D	C
	ATOM	7224	O	ALA	264	-4.451	-87.281	144.940	1.00	18.52	D	O
45	ATOM	7225	N	MET	265	-5.193	-85.707	143.517	1.00	18.79	D	N
	ATOM	7226	CA	MET	265	-3.890	-85.582	142.881	1.00	20.11	D	C
	ATOM	7227	CB	MET	265	-3.980	-84.685	141.642	1.00	21.94	D	C
	ATOM	7228	CG	MET	265	-4.664	-85.372	140.467	1.00	23.98	D	C
	ATOM	7229	SD	MET	265	-4.834	-84.332	139.013	1.00	27.16	D	S
50	ATOM	7230	CE	MET	265	-3.135	-84.314	138.431	1.00	25.04	D	C
	ATOM	7231	C	MET	265	-2.857	-85.057	143.868	1.00	19.34	D	C
	ATOM	7232	O	MET	265	-1.713	-85.486	143.850	1.00	18.51	D	O
	ATOM	7233	N	ALA	266	-3.263	-84.132	144.732	1.00	19.42	D	N
	ATOM	7234	CA	ALA	266	-2.359	-83.595	145.745	1.00	20.06	D	C
55	ATOM	7235	CB	ALA	266	-3.004	-82.389	146.444	1.00	19.09	D	C
	ATOM	7236	C	ALA	266	-2.089	-84.712	146.762	1.00	20.30	D	C
	ATOM	7237	O	ALA	266	-0.956	-84.919	147.200	1.00	19.06	D	O
	ATOM	7238	N	LEU	267	-3.147	-85.431	147.125	1.00	20.96	D	N
	ATOM	7239	CA	LEU	267	-3.049	-86.533	148.080	1.00	23.47	D	C
	ATOM	7240	CB	LEU	267	-4.409	-87.235	148.225	1.00	23.12	D	C
	ATOM	7241	CG	LEU	267	-4.784	-87.899	149.565	1.00	23.70	D	C
	ATOM	7242	CD1	LEU	267	-5.453	-89.234	149.295	1.00	21.48	D	C

-294-

	ATOM	7243	CD2	LEU	267	-3.568	-88.082	150.449	1.00	22.95	D	C
	ATOM	7244	C	LEU	267	-2.006	-87.564	147.648	1.00	23.83	D	C
	ATOM	7245	O	LEU	267	-1.107	-87.902	148.412	1.00	23.92	D	O
5	ATOM	7246	N	PHE	268	-2.118	-88.050	146.416	1.00	25.59	D	N
	ATOM	7247	CA	PHE	268	-1.193	-89.066	145.916	1.00	27.95	D	C
	ATOM	7248	CB	PHE	268	-1.936	-90.039	144.988	1.00	26.41	D	C
	ATOM	7249	CG	PHE	268	-3.071	-90.769	145.657	1.00	25.14	D	C
	ATOM	7250	CD1	PHE	268	-4.387	-90.525	145.286	1.00	24.11	D	C
10	ATOM	7251	CD2	PHE	268	-2.822	-91.688	146.676	1.00	25.38	D	C
	ATOM	7252	CE1	PHE	268	-5.438	-91.176	145.916	1.00	23.69	D	C
	ATOM	7253	CE2	PHE	268	-3.874	-92.351	147.318	1.00	23.66	D	C
	ATOM	7254	CZ	PHE	268	-5.180	-92.093	146.938	1.00	23.71	D	C
	ATOM	7255	C	PHE	268	0.072	-88.558	145.222	1.00	30.43	D	C
15	ATOM	7256	O	PHE	268	0.322	-88.862	144.057	1.00	30.67	D	O
	ATOM	7257	N	SER	269	0.871	-87.787	145.948	1.00	33.96	D	N
	ATOM	7258	CA	SER	269	2.129	-87.277	145.422	1.00	37.03	D	C
	ATOM	7259	CB	SER	269	2.419	-85.877	145.973	1.00	37.39	D	C
	ATOM	7260	OG	SER	269	1.497	-84.924	145.463	1.00	38.30	D	O
20	ATOM	7261	C	SER	269	3.192	-88.264	145.896	1.00	39.10	D	C
	ATOM	7262	O	SER	269	3.421	-88.411	147.096	1.00	38.72	D	O
	ATOM	7263	N	PRO	270	3.843	-88.969	144.954	1.00	41.49	D	N
	ATOM	7264	CD	PRO	270	3.602	-88.913	143.499	1.00	41.60	D	C
	ATOM	7265	CA	PRO	270	4.884	-89.957	145.270	1.00	43.13	D	C
25	ATOM	7266	CB	PRO	270	5.051	-90.704	143.951	1.00	42.69	D	C
	ATOM	7267	CG	PRO	270	4.821	-89.621	142.940	1.00	42.36	D	C
	ATOM	7268	C	PRO	270	6.211	-89.397	145.782	1.00	44.56	D	C
	ATOM	7269	O	PRO	270	7.015	-90.131	146.361	1.00	45.15	D	O
	ATOM	7270	N	ASP	271	6.441	-88.105	145.577	1.00	45.55	D	N
30	ATOM	7271	CA	ASP	271	7.687	-87.482	146.010	1.00	46.83	D	C
	ATOM	7272	CB	ASP	271	8.101	-86.413	144.996	1.00	48.20	D	C
	ATOM	7273	CG	ASP	271	7.070	-85.312	144.852	1.00	49.90	D	C
	ATOM	7274	OD1	ASP	271	5.860	-85.620	144.759	1.00	50.47	D	O
	ATOM	7275	OD2	ASP	271	7.475	-84.131	144.818	1.00	50.92	D	O
35	ATOM	7276	C	ASP	271	7.636	-86.886	147.418	1.00	47.00	D	C
	ATOM	7277	O	ASP	271	8.521	-86.124	147.815	1.00	47.50	D	O
	ATOM	7278	N	ARG	272	6.602	-87.243	148.172	1.00	46.37	D	N
	ATOM	7279	CA	ARG	272	6.436	-86.762	149.534	1.00	45.93	D	C
	ATOM	7280	CB	ARG	272	5.047	-87.143	150.050	1.00	45.63	D	C
40	ATOM	7281	CG	ARG	272	4.218	-85.980	150.556	1.00	44.83	D	C
	ATOM	7282	CD	ARG	272	3.300	-85.410	149.482	1.00	42.90	D	C
	ATOM	7283	NE	ARG	272	3.425	-83.961	149.425	1.00	41.67	D	N
	ATOM	7284	CZ	ARG	272	2.515	-83.123	148.936	1.00	40.40	D	C
	ATOM	7285	NH1	ARG	272	1.366	-83.563	148.445	1.00	38.84	D	N
	ATOM	7286	NH2	ARG	272	2.770	-81.826	148.939	1.00	40.16	D	N
45	ATOM	7287	C	ARG	272	7.501	-87.396	150.435	1.00	46.08	D	C
	ATOM	7288	O	ARG	272	7.880	-88.555	150.246	1.00	45.78	D	O
	ATOM	7289	N	PRO	273	8.002	-86.644	151.428	1.00	46.22	D	N
	ATOM	7290	CD	PRO	273	7.752	-85.221	151.712	1.00	45.76	D	C
50	ATOM	7291	CA	PRO	273	9.023	-87.183	152.334	1.00	46.41	D	C
	ATOM	7292	CB	PRO	273	9.459	-85.954	153.132	1.00	46.21	D	C
	ATOM	7293	CG	PRO	273	8.237	-85.099	153.133	1.00	46.57	D	C
	ATOM	7294	C	PRO	273	8.513	-88.312	153.233	1.00	46.69	D	C
	ATOM	7295	O	PRO	273	7.513	-88.160	153.938	1.00	46.36	D	O
	ATOM	7296	N	GLY	274	9.205	-89.447	153.193	1.00	46.90	D	N
55	ATOM	7297	CA	GLY	274	8.817	-90.582	154.010	1.00	47.62	D	C
	ATOM	7298	C	GLY	274	7.962	-91.626	153.314	1.00	48.15	D	C
	ATOM	7299	O	GLY	274	7.498	-92.575	153.951	1.00	48.17	D	O
	ATOM	7300	N	VAL	275	7.748	-91.462	152.012	1.00	48.62	D	N

-295-

5	ATOM	7301	CA	VAL	275	6.938	-92.411	151.259	1.00	49.05	D	C
	ATOM	7302	CB	VAL	275	6.392	-91.779	149.953	1.00	48.86	D	C
	ATOM	7303	CG1	VAL	275	5.673	-92.833	149.121	1.00	48.34	D	C
	ATOM	7304	CG2	VAL	275	5.440	-90.640	150.289	1.00	47.97	D	C
	ATOM	7305	C	VAL	275	7.726	-93.669	150.913	1.00	49.50	D	C
10	ATOM	7306	O	VAL	275	8.835	-93.599	150.386	1.00	49.51	D	O
	ATOM	7307	N	THR	276	7.136	-94.818	151.224	1.00	50.30	D	N
	ATOM	7308	CA	THR	276	7.748	-96.112	150.957	1.00	51.08	D	C
	ATOM	7309	CB	THR	276	7.258	-97.168	151.975	1.00	51.15	D	C
	ATOM	7310	OG1	THR	276	7.755	-96.838	153.277	1.00	51.62	D	O
15	ATOM	7311	CG2	THR	276	7.742	-98.559	151.590	1.00	51.91	D	C
	ATOM	7312	C	THR	276	7.425	-96.590	149.542	1.00	51.59	D	C
	ATOM	7313	O	THR	276	8.321	-96.729	148.710	1.00	52.05	D	O
	ATOM	7314	N	GLN	277	6.144	-96.836	149.278	1.00	51.49	D	N
	ATOM	7315	CA	GLN	277	5.694	-97.304	147.973	1.00	51.75	D	C
20	ATOM	7316	CB	GLN	277	4.354	-98.023	148.118	1.00	52.32	D	C
	ATOM	7317	CG	GLN	277	4.459	-99.373	148.796	1.00	53.71	D	C
	ATOM	7318	CD	GLN	277	3.126	-100.079	148.880	1.00	54.80	D	C
	ATOM	7319	OE1	GLN	277	2.317	-100.020	147.951	1.00	55.58	D	O
	ATOM	7320	NE2	GLN	277	2.893	-100.768	149.988	1.00	55.24	D	N
25	ATOM	7321	C	GLN	277	5.568	-96.180	146.946	1.00	51.46	D	C
	ATOM	7322	O	GLN	277	4.477	-95.884	146.460	1.00	51.02	D	O
	ATOM	7323	N	ARG	278	6.700	-95.569	146.615	1.00	51.45	D	N
	ATOM	7324	CA	ARG	278	6.752	-94.475	145.654	1.00	51.57	D	C
	ATOM	7325	CB	ARG	278	8.207	-94.012	145.504	1.00	52.92	D	C
30	ATOM	7326	CG	ARG	278	8.501	-93.073	144.340	1.00	55.26	D	C
	ATOM	7327	CD	ARG	278	8.770	-93.845	143.046	1.00	57.26	D	C
	ATOM	7328	NE	ARG	278	9.472	-93.037	142.049	1.00	58.68	D	N
	ATOM	7329	CZ	ARG	278	10.736	-92.627	142.159	1.00	59.43	D	C
	ATOM	7330	NH1	ARG	278	11.461	-92.945	143.228	1.00	59.27	D	N
35	ATOM	7331	NH2	ARG	278	11.279	-91.892	141.194	1.00	59.72	D	N
	ATOM	7332	C	ARG	278	6.161	-94.846	144.296	1.00	50.85	D	C
	ATOM	7333	O	ARG	278	5.432	-94.059	143.693	1.00	50.65	D	O
	ATOM	7334	N	ASP	279	6.473	-96.046	143.821	1.00	50.22	D	N
	ATOM	7335	CA	ASP	279	5.982	-96.516	142.532	1.00	49.17	D	C
40	ATOM	7336	CB	ASP	279	6.693	-97.818	142.151	1.00	51.29	D	C
	ATOM	7337	CG	ASP	279	8.109	-97.585	141.643	1.00	53.01	D	C
	ATOM	7338	OD1	ASP	279	8.825	-96.739	142.221	1.00	54.57	D	O
	ATOM	7339	OD2	ASP	279	8.510	-98.254	140.667	1.00	54.28	D	O
	ATOM	7340	C	ASP	279	4.470	-96.718	142.508	1.00	47.62	D	C
45	ATOM	7341	O	ASP	279	3.801	-96.316	141.560	1.00	47.32	D	O
	ATOM	7342	N	GLU	280	3.931	-97.343	143.548	1.00	46.06	D	N
	ATOM	7343	CA	GLU	280	2.495	-97.579	143.622	1.00	44.64	D	C
	ATOM	7344	CB	GLU	280	2.157	-98.466	144.826	1.00	45.89	D	C
	ATOM	7345	CG	GLU	280	2.755	-99.866	144.754	1.00	48.45	D	C
50	ATOM	7346	CD	GLU	280	4.074	-99.997	145.509	1.00	49.73	D	C
	ATOM	7347	OE1	GLU	280	4.986	-99.165	145.302	1.00	49.56	D	O
	ATOM	7348	OE2	GLU	280	4.199	-100.947	146.312	1.00	51.25	D	O
	ATOM	7349	C	GLU	280	1.728	-96.260	143.715	1.00	42.74	D	C
	ATOM	7350	O	GLU	280	0.715	-96.074	143.045	1.00	42.04	D	O
55	ATOM	7351	N	ILE	281	2.213	-95.348	144.550	1.00	41.01	D	N
	ATOM	7352	CA	ILE	281	1.566	-94.053	144.706	1.00	40.02	D	C
	ATOM	7353	CB	ILE	281	2.166	-93.277	145.900	1.00	39.33	D	C
	ATOM	7354	CG2	ILE	281	1.636	-91.847	145.919	1.00	38.82	D	C
	ATOM	7355	CG1	ILE	281	1.807	-93.997	147.206	1.00	38.81	D	C
	ATOM	7356	CD1	ILE	281	2.431	-93.392	148.443	1.00	37.90	D	C
	ATOM	7357	C	ILE	281	1.694	-93.231	143.420	1.00	39.83	D	C
	ATOM	7358	O	ILE	281	0.794	-92.466	143.069	1.00	39.50	D	O

-296-

	ATOM	7359	N	ASP	282	2.810	-93.405	142.718	1.00	39.49	D	N
	ATOM	7360	CA	ASP	282	3.049	-92.698	141.465	1.00	39.92	D	C
	ATOM	7361	CB	ASP	282	4.440	-93.042	140.924	1.00	42.08	D	C
	ATOM	7362	CG	ASP	282	4.997	-91.967	140.010	1.00	44.33	D	C
5	ATOM	7363	OD1	ASP	282	4.385	-91.694	138.956	1.00	45.27	D	O
	ATOM	7364	OD2	ASP	282	6.053	-91.388	140.351	1.00	46.09	D	O
	ATOM	7365	C	ASP	282	1.977	-93.115	140.453	1.00	39.04	D	C
	ATOM	7366	O	ASP	282	1.403	-92.273	139.762	1.00	38.00	D	O
10	ATOM	7367	N	GLN	283	1.700	-94.417	140.385	1.00	38.52	D	N
	ATOM	7368	CA	GLN	283	0.691	-94.943	139.471	1.00	38.31	D	C
	ATOM	7369	CB	GLN	283	0.725	-96.476	139.448	1.00	40.70	D	C
	ATOM	7370	CG	GLN	283	2.066	-97.085	139.041	1.00	44.18	D	C
	ATOM	7371	CD	GLN	283	1.955	-98.564	138.677	1.00	46.41	D	C
	ATOM	7372	OE1	GLN	283	1.349	-99.354	139.404	1.00	47.67	D	O
15	ATOM	7373	NE2	GLN	283	2.546	-98.941	137.546	1.00	46.87	D	N
	ATOM	7374	C	GLN	283	-0.709	-94.475	139.860	1.00	36.85	D	C
	ATOM	7375	O	GLN	283	-1.567	-94.268	139.000	1.00	36.29	D	O
	ATOM	7376	N	LEU	284	-0.945	-94.321	141.159	1.00	35.69	D	N
20	ATOM	7377	CA	LEU	284	-2.249	-93.865	141.624	1.00	34.25	D	C
	ATOM	7378	CB	LEU	284	-2.346	-93.955	143.153	1.00	33.82	D	C
	ATOM	7379	CG	LEU	284	-2.472	-95.364	143.747	1.00	33.47	D	C
	ATOM	7380	CD1	LEU	284	-2.597	-95.281	145.259	1.00	32.83	D	C
	ATOM	7381	CD2	LEU	284	-3.696	-96.053	143.164	1.00	32.79	D	C
25	ATOM	7382	C	LEU	284	-2.483	-92.430	141.171	1.00	33.26	D	C
	ATOM	7383	O	LEU	284	-3.593	-92.069	140.781	1.00	31.51	D	O
	ATOM	7384	N	GLN	285	-1.435	-91.611	141.216	1.00	33.02	D	N
	ATOM	7385	CA	GLN	285	-1.570	-90.224	140.794	1.00	33.96	D	C
	ATOM	7386	CB	GLN	285	-0.281	-89.442	141.037	1.00	34.10	D	C
	ATOM	7387	CG	GLN	285	-0.430	-87.960	140.713	1.00	35.79	D	C
30	ATOM	7388	CD	GLN	285	0.792	-87.162	141.077	1.00	36.64	D	C
	ATOM	7389	OE1	GLN	285	1.848	-87.307	140.461	1.00	38.71	D	O
	ATOM	7390	NE2	GLN	285	0.665	-86.317	142.095	1.00	36.76	D	N
	ATOM	7391	C	GLN	285	-1.929	-90.141	139.317	1.00	33.52	D	C
	ATOM	7392	O	GLN	285	-2.799	-89.366	138.923	1.00	33.70	D	O
35	ATOM	7393	N	GLU	286	-1.258	-90.942	138.501	1.00	33.33	D	N
	ATOM	7394	CA	GLU	286	-1.522	-90.936	137.069	1.00	34.29	D	C
	ATOM	7395	CB	GLU	286	-0.568	-91.902	136.358	1.00	36.73	D	C
	ATOM	7396	CG	GLU	286	0.880	-91.694	136.801	1.00	41.05	D	C
	ATOM	7397	CD	GLU	286	1.897	-92.388	135.919	1.00	44.06	D	C
40	ATOM	7398	OE1	GLU	286	1.725	-93.594	135.629	1.00	46.05	D	O
	ATOM	7399	OE2	GLU	286	2.882	-91.724	135.525	1.00	45.70	D	O
	ATOM	7400	C	GLU	286	-2.976	-91.306	136.817	1.00	32.71	D	C
	ATOM	7401	O	GLU	286	-3.628	-90.726	135.951	1.00	31.80	D	O
	ATOM	7402	N	GLU	287	-3.486	-92.259	137.593	1.00	32.21	D	N
45	ATOM	7403	CA	GLU	287	-4.876	-92.683	137.467	1.00	31.48	D	C
	ATOM	7404	CB	GLU	287	-5.186	-93.841	138.421	1.00	33.15	D	C
	ATOM	7405	CG	GLU	287	-6.573	-94.430	138.208	1.00	36.26	D	C
	ATOM	7406	CD	GLU	287	-6.975	-95.435	139.278	1.00	38.20	D	C
	ATOM	7407	OE1	GLU	287	-6.145	-96.301	139.634	1.00	38.75	D	O
50	ATOM	7408	OE2	GLU	287	-8.131	-95.363	139.752	1.00	38.76	D	O
	ATOM	7409	C	GLU	287	-5.796	-91.517	137.787	1.00	29.64	D	C
	ATOM	7410	O	GLU	287	-6.812	-91.323	137.122	1.00	30.00	D	O
	ATOM	7411	N	MET	288	-5.451	-90.748	138.818	1.00	28.15	D	N
55	ATOM	7412	CA	MET	288	-6.258	-89.589	139.197	1.00	27.18	D	C
	ATOM	7413	CB	MET	288	-5.701	-88.916	140.464	1.00	26.96	D	C
	ATOM	7414	CG	MET	288	-5.579	-89.800	141.706	1.00	26.67	D	C
	ATOM	7415	SD	MET	288	-7.136	-90.501	142.292	1.00	26.45	D	S
	ATOM	7416	CE	MET	288	-6.849	-92.264	141.971	1.00	27.72	D	C

-297-

	ATOM	7417	C	MET	288	-6.207	-88.592	138.040	1.00	26.19	D	C
	ATOM	7418	O	MET	288	-7.231	-88.074	137.607	1.00	25.68	D	O
	ATOM	7419	N	ALA	289	-4.999	-88.348	137.539	1.00	25.78	D	N
5	ATOM	7420	CA	ALA	289	-4.771	-87.407	136.440	1.00	25.91	D	C
	ATOM	7421	CB	ALA	289	-3.276	-87.358	136.108	1.00	24.39	D	C
	ATOM	7422	C	ALA	289	-5.580	-87.746	135.185	1.00	25.97	D	C
	ATOM	7423	O	ALA	289	-6.245	-86.883	134.605	1.00	25.73	D	O
	ATOM	7424	N	LEU	290	-5.526	-89.003	134.765	1.00	26.73	D	N
10	ATOM	7425	CA	LEU	290	-6.260	-89.423	133.585	1.00	27.49	D	C
	ATOM	7426	CB	LEU	290	-5.920	-90.873	133.238	1.00	30.25	D	C
	ATOM	7427	CG	LEU	290	-4.511	-91.055	132.662	1.00	31.14	D	C
	ATOM	7428	CD1	LEU	290	-4.257	-92.519	132.347	1.00	32.31	D	C
	ATOM	7429	CD2	LEU	290	-4.383	-90.217	131.402	1.00	32.28	D	C
15	ATOM	7430	C	LEU	290	-7.759	-89.265	133.767	1.00	26.79	D	C
	ATOM	7431	O	LEU	290	-8.458	-88.847	132.845	1.00	26.47	D	O
	ATOM	7432	N	THR	291	-8.255	-89.596	134.955	1.00	25.93	D	N
	ATOM	7433	CA	THR	291	-9.683	-89.466	135.231	1.00	25.58	D	C
	ATOM	7434	CB	THR	291	-10.017	-89.994	136.638	1.00	25.08	D	C
20	ATOM	7435	OG1	THR	291	-9.603	-91.361	136.735	1.00	24.28	D	O
	ATOM	7436	CG2	THR	291	-11.502	-89.905	136.912	1.00	24.63	D	C
	ATOM	7437	C	THR	291	-10.112	-88.003	135.112	1.00	25.32	D	C
	ATOM	7438	O	THR	291	-11.170	-87.702	134.558	1.00	25.11	D	O
	ATOM	7439	N	LEU	292	-9.292	-87.097	135.639	1.00	25.55	D	N
25	ATOM	7440	CA	LEU	292	-9.582	-85.668	135.559	1.00	26.33	D	C
	ATOM	7441	CB	LEU	292	-8.542	-84.857	136.344	1.00	25.09	D	C
	ATOM	7442	CG	LEU	292	-8.601	-83.329	136.197	1.00	24.67	D	C
	ATOM	7443	CD1	LEU	292	-10.006	-82.825	136.510	1.00	23.71	D	C
	ATOM	7444	CD2	LEU	292	-7.579	-82.682	137.130	1.00	23.44	D	C
30	ATOM	7445	C	LEU	292	-9.582	-85.217	134.099	1.00	27.35	D	C
	ATOM	7446	O	LEU	292	-10.476	-84.492	133.670	1.00	26.47	D	O
	ATOM	7447	N	GLN	293	-8.568	-85.638	133.344	1.00	29.48	D	N
	ATOM	7448	CA	GLN	293	-8.471	-85.281	131.928	1.00	32.08	D	C
	ATOM	7449	CB	GLN	293	-7.219	-85.901	131.301	1.00	34.17	D	C
35	ATOM	7450	CG	GLN	293	-5.911	-85.424	131.910	1.00	37.03	D	C
	ATOM	7451	CD	GLN	293	-4.706	-86.160	131.347	1.00	39.59	D	C
	ATOM	7452	OE1	GLN	293	-4.504	-86.205	130.129	1.00	41.51	D	O
	ATOM	7453	NE2	GLN	293	-3.897	-86.743	132.232	1.00	40.22	D	N
	ATOM	7454	C	GLN	293	-9.708	-85.788	131.198	1.00	32.47	D	C
40	ATOM	7455	O	GLN	293	-10.365	-85.034	130.489	1.00	31.68	D	O
	ATOM	7456	N	SER	294	-10.019	-87.069	131.386	1.00	33.78	D	N
	ATOM	7457	CA	SER	294	-11.187	-87.688	130.760	1.00	35.43	D	C
	ATOM	7458	CB	SER	294	-11.302	-89.151	131.185	1.00	35.97	D	C
	ATOM	7459	OG	SER	294	-10.173	-89.898	130.763	1.00	38.15	D	O
45	ATOM	7460	C	SER	294	-12.472	-86.955	131.130	1.00	35.91	D	C
	ATOM	7461	O	SER	294	-13.335	-86.722	130.282	1.00	36.34	D	O
	ATOM	7462	N	TYR	295	-12.608	-86.599	132.400	1.00	35.87	D	N
	ATOM	7463	CA	TYR	295	-13.797	-85.889	132.830	1.00	36.69	D	C
	ATOM	7464	CB	TYR	295	-13.784	-85.698	134.350	1.00	35.73	D	C
	ATOM	7465	CG	TYR	295	-14.957	-84.903	134.855	1.00	34.69	D	C
50	ATOM	7466	CD1	TYR	295	-14.937	-83.512	134.827	1.00	34.72	D	C
	ATOM	7467	CE1	TYR	295	-16.037	-82.768	135.226	1.00	34.93	D	C
	ATOM	7468	CD2	TYR	295	-16.115	-85.538	135.304	1.00	35.18	D	C
	ATOM	7469	CE2	TYR	295	-17.226	-84.805	135.706	1.00	34.88	D	C
55	ATOM	7470	CZ	TYR	295	-17.180	-83.417	135.662	1.00	35.17	D	C
	ATOM	7471	OH	TYR	295	-18.273	-82.672	136.034	1.00	35.12	D	O
	ATOM	7472	C	TYR	295	-13.894	-84.538	132.119	1.00	37.83	D	C
	ATOM	7473	O	TYR	295	-14.966	-84.156	131.651	1.00	37.60	D	O
	ATOM	7474	N	ILE	296	-12.777	-83.818	132.040	1.00	39.36	D	N

-298-

	ATOM	7475	CA	ILE	296	-12.745	-82.514	131.377	1.00	41.08	D	C
	ATOM	7476	CB	ILE	296	-11.348	-81.833	131.526	1.00	40.29	D	C
	ATOM	7477	CG2	ILE	296	-11.266	-80.591	130.637	1.00	39.62	D	C
5	ATOM	7478	CG1	ILE	296	-11.105	-81.446	132.993	1.00	39.58	D	C
	ATOM	7479	CD1	ILE	296	-9.736	-80.836	133.259	1.00	37.65	D	C
	ATOM	7480	C	ILE	296	-13.091	-82.651	129.889	1.00	42.83	D	C
	ATOM	7481	O	ILE	296	-13.844	-81.844	129.347	1.00	42.30	D	O
	ATOM	7482	N	LYS	297	-12.535	-83.673	129.239	1.00	45.50	D	N
10	ATOM	7483	CA	LYS	297	-12.792	-83.929	127.821	1.00	48.44	D	C
	ATOM	7484	CB	LYS	297	-11.960	-85.114	127.325	1.00	48.12	D	C
	ATOM	7485	CG	LYS	297	-10.472	-84.861	127.207	1.00	48.26	D	C
	ATOM	7486	CD	LYS	297	-9.791	-86.096	126.643	1.00	49.23	D	C
	ATOM	7487	CE	LYS	297	-8.297	-85.891	126.458	1.00	50.24	D	C
	ATOM	7488	NZ	LYS	297	-7.652	-87.102	125.872	1.00	50.73	D	N
15	ATOM	7489	C	LYS	297	-14.264	-84.245	127.600	1.00	50.60	D	C
	ATOM	7490	O	LYS	297	-14.903	-83.690	126.707	1.00	50.62	D	O
	ATOM	7491	N	GLY	298	-14.793	-85.151	128.415	1.00	53.71	D	N
	ATOM	7492	CA	GLY	298	-16.187	-85.527	128.300	1.00	57.58	D	C
20	ATOM	7493	C	GLY	298	-17.093	-84.372	128.665	1.00	60.34	D	C
	ATOM	7494	O	GLY	298	-17.583	-83.664	127.794	1.00	60.81	D	O
	ATOM	7495	N	GLN	299	-17.308	-84.180	129.960	1.00	63.65	D	N
	ATOM	7496	CA	GLN	299	-18.163	-83.108	130.453	1.00	66.89	D	C
	ATOM	7497	CB	GLN	299	-18.154	-83.099	131.988	1.00	67.10	D	C
	ATOM	7498	CG	GLN	299	-19.240	-82.244	132.644	1.00	68.11	D	C
25	ATOM	7499	CD	GLN	299	-19.157	-80.773	132.268	1.00	68.71	D	C
	ATOM	7500	OE1	GLN	299	-18.097	-80.153	132.367	1.00	69.05	D	O
	ATOM	7501	NE2	GLN	299	-20.283	-80.205	131.844	1.00	69.38	D	N
	ATOM	7502	C	GLN	299	-17.716	-81.745	129.926	1.00	68.91	D	C
30	ATOM	7503	O	GLN	299	-16.739	-81.171	130.411	1.00	69.02	D	O
	ATOM	7504	N	GLN	300	-18.440	-81.239	128.931	1.00	71.20	D	N
	ATOM	7505	CA	GLN	300	-18.152	-79.938	128.336	1.00	73.67	D	C
	ATOM	7506	CB	GLN	300	-16.696	-79.872	127.836	1.00	74.21	D	C
	ATOM	7507	CG	GLN	300	-16.254	-81.023	126.939	1.00	75.16	D	C
	ATOM	7508	CD	GLN	300	-15.178	-80.605	125.951	1.00	75.58	D	C
35	ATOM	7509	OE1	GLN	300	-14.091	-80.174	126.340	1.00	75.70	D	O
	ATOM	7510	NE2	GLN	300	-15.482	-80.726	124.662	1.00	75.83	D	N
	ATOM	7511	C	GLN	300	-19.132	-79.598	127.203	1.00	74.94	D	C
	ATOM	7512	O	GLN	300	-20.325	-79.410	127.454	1.00	75.30	D	O
40	ATOM	7513	N	ARG	301	-18.624	-79.518	125.972	1.00	76.23	D	N
	ATOM	7514	CA	ARG	301	-19.407	-79.191	124.775	1.00	77.42	D	C
	ATOM	7515	CB	ARG	301	-20.718	-79.989	124.734	1.00	77.89	D	C
	ATOM	7516	CG	ARG	301	-21.380	-80.038	123.354	1.00	78.74	D	C
	ATOM	7517	CD	ARG	301	-20.655	-80.989	122.388	1.00	79.60	D	C
	ATOM	7518	NE	ARG	301	-19.295	-80.558	122.053	1.00	79.99	D	N
45	ATOM	7519	CZ	ARG	301	-18.991	-79.600	121.181	1.00	80.24	D	C
	ATOM	7520	NH1	ARG	301	-19.948	-78.952	120.529	1.00	80.26	D	N
	ATOM	7521	NH2	ARG	301	-17.721	-79.280	120.969	1.00	80.28	D	N
	ATOM	7522	C	ARG	301	-19.706	-77.692	124.705	1.00	77.75	D	C
	ATOM	7523	O	ARG	301	-19.729	-77.099	123.624	1.00	78.10	D	O
50	ATOM	7524	N	ARG	302	-19.938	-77.091	125.868	1.00	77.90	D	N
	ATOM	7525	CA	ARG	302	-20.208	-75.664	125.980	1.00	77.67	D	C
	ATOM	7526	CB	ARG	302	-21.356	-75.402	126.965	1.00	78.48	D	C
	ATOM	7527	CG	ARG	302	-22.504	-76.403	126.880	1.00	79.56	D	C
	ATOM	7528	CD	ARG	302	-23.259	-76.320	125.564	1.00	80.20	D	C
55	ATOM	7529	NE	ARG	302	-24.087	-77.507	125.360	1.00	81.19	D	N
	ATOM	7530	CZ	ARG	302	-25.097	-77.587	124.499	1.00	81.77	D	C
	ATOM	7531	NH1	ARG	302	-25.425	-76.542	123.749	1.00	81.87	D	N
	ATOM	7532	NH2	ARG	302	-25.779	-78.720	124.386	1.00	81.98	D	N

-299-

	ATOM	7533	C	ARG	302	-18.911	-75.032	126.498	1.00	76.83	D	C
	ATOM	7534	O	ARG	302	-18.303	-74.206	125.812	1.00	77.05	D	O
	ATOM	7535	N	PRO	303	-18.459	-75.423	127.711	1.00	75.72	D	N
	ATOM	7536	CD	PRO	303	-18.978	-76.402	128.687	1.00	75.41	D	C
5	ATOM	7537	CA	PRO	303	-17.215	-74.820	128.201	1.00	74.46	D	C
	ATOM	7538	CB	PRO	303	-16.951	-75.576	129.505	1.00	74.67	D	C
	ATOM	7539	CG	PRO	303	-18.322	-75.955	129.968	1.00	75.17	D	C
	ATOM	7540	C	PRO	303	-16.100	-75.043	127.180	1.00	73.06	D	C
10	ATOM	7541	O	PRO	303	-15.406	-74.104	126.783	1.00	73.11	D	O
	ATOM	7542	N	ARG	304	-15.962	-76.298	126.753	1.00	71.01	D	N
	ATOM	7543	CA	ARG	304	-14.947	-76.711	125.791	1.00	68.70	D	C
	ATOM	7544	CB	ARG	304	-15.518	-76.711	124.369	1.00	69.88	D	C
	ATOM	7545	CG	ARG	304	-14.832	-77.704	123.428	1.00	71.21	D	C
	ATOM	7546	CD	ARG	304	-13.434	-77.252	123.009	1.00	72.37	D	C
15	ATOM	7547	NE	ARG	304	-12.645	-78.321	122.386	1.00	73.31	D	N
	ATOM	7548	CZ	ARG	304	-12.957	-78.953	121.254	1.00	73.71	D	C
	ATOM	7549	NH1	ARG	304	-14.059	-78.645	120.578	1.00	74.08	D	N
	ATOM	7550	NH2	ARG	304	-12.155	-79.904	120.792	1.00	73.93	D	N
	ATOM	7551	C	ARG	304	-13.725	-75.809	125.869	1.00	66.18	D	C
20	ATOM	7552	O	ARG	304	-13.540	-74.904	125.054	1.00	66.00	D	O
	ATOM	7553	N	ASP	305	-12.906	-76.055	126.884	1.00	63.00	D	N
	ATOM	7554	CA	ASP	305	-11.689	-75.292	127.091	1.00	59.34	D	C
	ATOM	7555	CB	ASP	305	-11.760	-74.528	128.414	1.00	59.31	D	C
	ATOM	7556	CG	ASP	305	-10.496	-73.749	128.703	1.00	59.38	D	C
25	ATOM	7557	OD1	ASP	305	-9.693	-73.556	127.766	1.00	59.54	D	O
	ATOM	7558	OD2	ASP	305	-10.308	-73.320	129.861	1.00	59.45	D	O
	ATOM	7559	C	ASP	305	-10.522	-76.270	127.100	1.00	56.66	D	C
	ATOM	7560	O	ASP	305	-10.363	-77.058	128.036	1.00	56.22	D	O
	ATOM	7561	N	ARG	306	-9.718	-76.227	126.042	1.00	52.93	D	N
30	ATOM	7562	CA	ARG	306	-8.569	-77.113	125.926	1.00	49.32	D	C
	ATOM	7563	CB	ARG	306	-8.043	-77.118	124.487	1.00	50.93	D	C
	ATOM	7564	CG	ARG	306	-8.942	-77.823	123.481	1.00	52.84	D	C
	ATOM	7565	CD	ARG	306	-8.225	-78.027	122.147	1.00	54.60	D	C
	ATOM	7566	NE	ARG	306	-7.878	-76.761	121.500	1.00	56.43	D	N
35	ATOM	7567	CZ	ARG	306	-8.754	-75.945	120.917	1.00	57.34	D	C
	ATOM	7568	NH1	ARG	306	-10.047	-76.251	120.887	1.00	58.29	D	N
	ATOM	7569	NH2	ARG	306	-8.336	-74.814	120.367	1.00	57.94	D	N
	ATOM	7570	C	ARG	306	-7.431	-76.756	126.879	1.00	45.59	D	C
	ATOM	7571	O	ARG	306	-6.527	-77.559	127.086	1.00	45.21	D	O
40	ATOM	7572	N	PHE	307	-7.474	-75.558	127.456	1.00	41.34	D	N
	ATOM	7573	CA	PHE	307	-6.431	-75.114	128.378	1.00	37.64	D	C
	ATOM	7574	CB	PHE	307	-6.214	-73.601	128.244	1.00	37.62	D	C
	ATOM	7575	CG	PHE	307	-5.764	-73.168	126.876	1.00	38.89	D	C
	ATOM	7576	CD1	PHE	307	-6.693	-72.895	125.872	1.00	38.94	D	C
45	ATOM	7577	CD2	PHE	307	-4.407	-73.060	126.580	1.00	38.30	D	C
	ATOM	7578	CE1	PHE	307	-6.276	-72.523	124.591	1.00	38.89	D	C
	ATOM	7579	CE2	PHE	307	-3.981	-72.689	125.305	1.00	38.37	D	C
	ATOM	7580	CZ	PHE	307	-4.918	-72.421	124.309	1.00	38.57	D	C
	ATOM	7581	C	PHE	307	-6.683	-75.442	129.855	1.00	34.77	D	C
50	ATOM	7582	O	PHE	307	-5.797	-75.259	130.692	1.00	33.68	D	O
	ATOM	7583	N	LEU	308	-7.878	-75.933	130.174	1.00	31.44	D	N
	ATOM	7584	CA	LEU	308	-8.233	-76.236	131.558	1.00	28.34	D	C
	ATOM	7585	CB	LEU	308	-9.653	-76.805	131.625	1.00	27.84	D	C
	ATOM	7586	CG	LEU	308	-10.526	-76.317	132.793	1.00	28.71	D	C
55	ATOM	7587	CD1	LEU	308	-11.726	-77.241	132.946	1.00	29.15	D	C
	ATOM	7588	CD2	LEU	308	-9.737	-76.288	134.081	1.00	26.96	D	C
	ATOM	7589	C	LEU	308	-7.274	-77.172	132.311	1.00	26.41	D	C
	ATOM	7590	O	LEU	308	-6.724	-76.797	133.345	1.00	24.44	D	O

-300-

5	ATOM	7591	N	TYR	309	-7.079	-78.385	131.810	1.00	24.84	D	N
	ATOM	7592	CA	TYR	309	-6.199	-79.333	132.489	1.00	24.89	D	C
	ATOM	7593	CB	TYR	309	-6.107	-80.634	131.691	1.00	24.35	D	C
	ATOM	7594	CG	TYR	309	-5.286	-81.708	132.373	1.00	25.38	D	C
	ATOM	7595	CD1	TYR	309	-5.667	-82.214	133.617	1.00	24.51	D	C
10	ATOM	7596	CE1	TYR	309	-4.922	-83.203	134.254	1.00	24.34	D	C
	ATOM	7597	CD2	TYR	309	-4.127	-82.220	131.778	1.00	24.33	D	C
	ATOM	7598	CE2	TYR	309	-3.372	-83.215	132.410	1.00	24.59	D	C
	ATOM	7599	CZ	TYR	309	-3.781	-83.698	133.650	1.00	24.77	D	C
	ATOM	7600	OH	TYR	309	-3.061	-84.683	134.288	1.00	25.73	D	O
15	ATOM	7601	C	TYR	309	-4.794	-78.774	132.732	1.00	24.60	D	C
	ATOM	7602	O	TYR	309	-4.249	-78.888	133.835	1.00	24.29	D	O
	ATOM	7603	N	ALA	310	-4.208	-78.171	131.703	1.00	23.83	D	N
	ATOM	7604	CA	ALA	310	-2.873	-77.601	131.826	1.00	23.53	D	C
	ATOM	7605	CB	ALA	310	-2.445	-76.970	130.498	1.00	22.84	D	C
20	ATOM	7606	C	ALA	310	-2.843	-76.562	132.948	1.00	22.76	D	C
	ATOM	7607	O	ALA	310	-1.902	-76.522	133.740	1.00	21.87	D	O
	ATOM	7608	N	LYS	311	-3.868	-75.715	133.010	1.00	22.43	D	N
	ATOM	7609	CA	LYS	311	-3.943	-74.707	134.063	1.00	22.75	D	C
	ATOM	7610	CB	LYS	311	-5.146	-73.782	133.858	1.00	23.52	D	C
25	ATOM	7611	CG	LYS	311	-4.926	-72.669	132.843	1.00	25.26	D	C
	ATOM	7612	CD	LYS	311	-6.227	-71.915	132.590	1.00	27.42	D	C
	ATOM	7613	CE	LYS	311	-6.022	-70.752	131.630	1.00	30.14	D	C
	ATOM	7614	NZ	LYS	311	-7.321	-70.118	131.265	1.00	32.77	D	N
	ATOM	7615	C	LYS	311	-4.039	-75.359	135.444	1.00	22.13	D	C
30	ATOM	7616	O	LYS	311	-3.433	-74.877	136.399	1.00	21.60	D	O
	ATOM	7617	N	LEU	312	-4.797	-76.450	135.547	1.00	20.89	D	N
	ATOM	7618	CA	LEU	312	-4.950	-77.139	136.823	1.00	21.30	D	C
	ATOM	7619	CB	LEU	312	-6.033	-78.219	136.726	1.00	20.26	D	C
	ATOM	7620	CG	LEU	312	-7.442	-77.639	136.538	1.00	20.91	D	C
35	ATOM	7621	CD1	LEU	312	-8.472	-78.737	136.375	1.00	19.59	D	C
	ATOM	7622	CD2	LEU	312	-7.775	-76.766	137.740	1.00	21.76	D	C
	ATOM	7623	C	LEU	312	-3.624	-77.737	137.292	1.00	21.85	D	C
	ATOM	7624	O	LEU	312	-3.320	-77.710	138.483	1.00	20.99	D	O
	ATOM	7625	N	LEU	313	-2.837	-78.280	136.365	1.00	20.96	D	N
40	ATOM	7626	CA	LEU	313	-1.539	-78.833	136.736	1.00	21.57	D	C
	ATOM	7627	CB	LEU	313	-0.866	-79.514	135.541	1.00	20.84	D	C
	ATOM	7628	CG	LEU	313	-1.525	-80.804	135.048	1.00	21.35	D	C
	ATOM	7629	CD1	LEU	313	-0.628	-81.462	134.016	1.00	19.73	D	C
	ATOM	7630	CD2	LEU	313	-1.765	-81.757	136.234	1.00	21.46	D	C
45	ATOM	7631	C	LEU	313	-0.668	-77.683	137.230	1.00	21.97	D	C
	ATOM	7632	O	LEU	313	0.088	-77.828	138.190	1.00	21.62	D	O
	ATOM	7633	N	GLY	314	-0.789	-76.533	136.573	1.00	22.24	D	N
	ATOM	7634	CA	GLY	314	-0.019	-75.377	136.980	1.00	22.60	D	C
	ATOM	7635	C	GLY	314	-0.403	-74.940	138.383	1.00	23.14	D	C
50	ATOM	7636	O	GLY	314	0.456	-74.597	139.198	1.00	22.01	D	O
	ATOM	7637	N	LEU	315	-1.702	-74.947	138.667	1.00	23.45	D	N
	ATOM	7638	CA	LEU	315	-2.182	-74.554	139.986	1.00	24.19	D	C
	ATOM	7639	CB	LEU	315	-3.706	-74.402	139.979	1.00	24.08	D	C
	ATOM	7640	CG	LEU	315	-4.171	-73.057	139.404	1.00	25.31	D	C
55	ATOM	7641	CD1	LEU	315	-5.668	-73.072	139.159	1.00	24.47	D	C
	ATOM	7642	CD2	LEU	315	-3.795	-71.932	140.383	1.00	24.52	D	C
	ATOM	7643	C	LEU	315	-1.741	-75.547	141.055	1.00	23.53	D	C
	ATOM	7644	O	LEU	315	-1.569	-75.169	142.213	1.00	23.85	D	O
	ATOM	7645	N	LEU	316	-1.552	-76.806	140.667	1.00	23.29	D	N
	ATOM	7646	CA	LEU	316	-1.095	-77.834	141.605	1.00	23.36	D	C
	ATOM	7647	CB	LEU	316	-1.196	-79.222	140.982	1.00	24.00	D	C
	ATOM	7648	CG	LEU	316	-2.589	-79.846	141.012	1.00	26.29	D	C

-301-

5	ATOM	7649	CD1	LEU	316	-2.533	-81.247	140.416	1.00	25.87	D	C
	ATOM	7650	CD2	LEU	316	-3.090	-79.904	142.453	1.00	25.54	D	C
	ATOM	7651	C	LEU	316	0.346	-77.572	142.028	1.00	22.98	D	C
	ATOM	7652	O	LEU	316	0.704	-77.776	143.189	1.00	22.32	D	O
	ATOM	7653	N	ALA	317	1.174	-77.134	141.079	1.00	22.45	D	N
10	ATOM	7654	CA	ALA	317	2.567	-76.815	141.374	1.00	22.43	D	C
	ATOM	7655	CB	ALA	317	3.355	-76.602	140.072	1.00	21.73	D	C
	ATOM	7656	C	ALA	317	2.599	-75.543	142.236	1.00	22.46	D	C
	ATOM	7657	O	ALA	317	3.393	-75.435	143.170	1.00	21.94	D	O
	ATOM	7658	N	GLU	318	1.736	-74.581	141.923	1.00	22.48	D	N
15	ATOM	7659	CA	GLU	318	1.681	-73.353	142.706	1.00	23.87	D	C
	ATOM	7660	CB	GLU	318	0.666	-72.364	142.122	1.00	25.70	D	C
	ATOM	7661	CG	GLU	318	0.508	-71.114	142.984	1.00	31.16	D	C
	ATOM	7662	CD	GLU	318	-0.110	-69.941	142.249	1.00	34.23	D	C
	ATOM	7663	OE1	GLU	318	-1.252	-70.057	141.761	1.00	36.85	D	O
20	ATOM	7664	OE2	GLU	318	0.553	-68.888	142.164	1.00	37.30	D	O
	ATOM	7665	C	GLU	318	1.297	-73.687	144.144	1.00	23.13	D	C
	ATOM	7666	O	GLU	318	1.880	-73.163	145.095	1.00	21.66	D	O
	ATOM	7667	N	LEU	319	0.314	-74.569	144.299	1.00	22.62	D	N
	ATOM	7668	CA	LEU	319	-0.130	-74.982	145.623	1.00	22.59	D	C
25	ATOM	7669	CB	LEU	319	-1.309	-75.953	145.491	1.00	22.32	D	C
	ATOM	7670	CG	LEU	319	-2.055	-76.411	146.743	1.00	22.65	D	C
	ATOM	7671	CD1	LEU	319	-2.451	-75.211	147.601	1.00	19.98	D	C
	ATOM	7672	CD2	LEU	319	-3.290	-77.207	146.314	1.00	21.48	D	C
	ATOM	7673	C	LEU	319	1.046	-75.647	146.349	1.00	22.54	D	C
30	ATOM	7674	O	LEU	319	1.216	-75.492	147.560	1.00	21.29	D	O
	ATOM	7675	N	ARG	320	1.860	-76.382	145.597	1.00	22.22	D	N
	ATOM	7676	CA	ARG	320	3.025	-77.044	146.163	1.00	23.46	D	C
	ATOM	7677	CB	ARG	320	3.699	-77.913	145.100	1.00	25.91	D	C
	ATOM	7678	CG	ARG	320	4.765	-78.840	145.639	1.00	29.09	D	C
35	ATOM	7679	CD	ARG	320	4.173	-79.913	146.542	1.00	32.17	D	C
	ATOM	7680	NE	ARG	320	5.219	-80.808	147.039	1.00	35.46	D	N
	ATOM	7681	CZ	ARG	320	5.452	-82.041	146.590	1.00	35.28	D	C
	ATOM	7682	NH1	ARG	320	4.712	-82.566	145.619	1.00	35.19	D	N
	ATOM	7683	NH2	ARG	320	6.439	-82.752	147.120	1.00	36.23	D	N
40	ATOM	7684	C	ARG	320	4.003	-75.985	146.675	1.00	22.95	D	C
	ATOM	7685	O	ARG	320	4.571	-76.127	147.758	1.00	22.89	D	O
	ATOM	7686	N	SER	321	4.208	-74.929	145.893	1.00	22.56	D	N
	ATOM	7687	CA	SER	321	5.094	-73.836	146.302	1.00	23.16	D	C
	ATOM	7688	CB	SER	321	5.182	-72.764	145.210	1.00	24.44	D	C
45	ATOM	7689	OG	SER	321	5.696	-73.299	144.004	1.00	29.71	D	O
	ATOM	7690	C	SER	321	4.546	-73.192	147.578	1.00	21.76	D	C
	ATOM	7691	O	SER	321	5.302	-72.835	148.477	1.00	21.35	D	O
	ATOM	7692	N	ILE	322	3.228	-73.040	147.648	1.00	20.52	D	N
	ATOM	7693	CA	ILE	322	2.599	-72.450	148.825	1.00	20.27	D	C
50	ATOM	7694	CB	ILE	322	1.079	-72.270	148.611	1.00	19.98	D	C
	ATOM	7695	CG2	ILE	322	0.389	-71.947	149.941	1.00	20.29	D	C
	ATOM	7696	CG1	ILE	322	0.849	-71.147	147.601	1.00	20.19	D	C
	ATOM	7697	CD1	ILE	322	-0.591	-70.931	147.197	1.00	21.36	D	C
	ATOM	7698	C	ILE	322	2.864	-73.316	150.054	1.00	19.11	D	C
55	ATOM	7699	O	ILE	322	3.200	-72.812	151.120	1.00	17.80	D	O
	ATOM	7700	N	ASN	323	2.732	-74.624	149.888	1.00	20.09	D	N
	ATOM	7701	CA	ASN	323	2.975	-75.574	150.972	1.00	20.89	D	C
	ATOM	7702	CB	ASN	323	2.811	-77.007	150.449	1.00	23.19	D	C
	ATOM	7703	CG	ASN	323	2.485	-78.011	151.556	1.00	26.69	D	C
	ATOM	7704	OD1	ASN	323	2.830	-79.192	151.453	1.00	28.16	D	O
	ATOM	7705	ND2	ASN	323	1.801	-77.553	152.602	1.00	26.88	D	N
	ATOM	7706	C	ASN	323	4.398	-75.369	151.511	1.00	20.52	D	C

-302-

	ATOM	7707	O	ASN	323	4.609	-75.346	152.718	1.00	18.86	D	O
	ATOM	7708	N	GLU	324	5.371	-75.227	150.610	1.00	20.84	D	N
	ATOM	7709	CA	GLU	324	6.763	-74.997	151.009	1.00	22.21	D	C
5	ATOM	7710	CB	GLU	324	7.689	-75.077	149.794	1.00	23.95	D	C
	ATOM	7711	CG	GLU	324	8.155	-76.472	149.463	1.00	27.94	D	C
	ATOM	7712	CD	GLU	324	8.511	-76.621	148.003	1.00	31.05	D	C
	ATOM	7713	OE1	GLU	324	9.069	-75.663	147.424	1.00	33.20	D	O
	ATOM	7714	OE2	GLU	324	8.238	-77.702	147.435	1.00	32.71	D	O
10	ATOM	7715	C	GLU	324	6.938	-73.630	151.671	1.00	21.32	D	C
	ATOM	7716	O	GLU	324	7.694	-73.490	152.633	1.00	20.59	D	O
	ATOM	7717	N	ALA	325	6.256	-72.619	151.140	1.00	20.62	D	N
	ATOM	7718	CA	ALA	325	6.339	-71.281	151.707	1.00	20.95	D	C
	ATOM	7719	CB	ALA	325	5.551	-70.298	150.853	1.00	20.62	D	C
15	ATOM	7720	C	ALA	325	5.795	-71.317	153.139	1.00	21.67	D	C
	ATOM	7721	O	ALA	325	6.271	-70.587	154.002	1.00	23.20	D	O
	ATOM	7722	N	TYR	326	4.802	-72.164	153.396	1.00	21.72	D	N
	ATOM	7723	CA	TYR	326	4.259	-72.285	154.747	1.00	22.87	D	C
	ATOM	7724	CB	TYR	326	3.150	-73.337	154.798	1.00	21.37	D	C
20	ATOM	7725	CG	TYR	326	1.745	-72.783	154.727	1.00	20.49	D	C
	ATOM	7726	CD1	TYR	326	1.246	-71.948	155.730	1.00	19.50	D	C
	ATOM	7727	CE1	TYR	326	-0.074	-71.498	155.701	1.00	18.19	D	C
	ATOM	7728	CD2	TYR	326	0.889	-73.145	153.689	1.00	19.15	D	C
	ATOM	7729	CE2	TYR	326	-0.422	-72.707	153.652	1.00	17.68	D	C
25	ATOM	7730	CZ	TYR	326	-0.901	-71.888	154.658	1.00	18.08	D	C
	ATOM	7731	OH	TYR	326	-2.220	-71.494	154.626	1.00	16.91	D	O
	ATOM	7732	C	TYR	326	5.392	-72.697	155.688	1.00	23.78	D	C
	ATOM	7733	O	TYR	326	5.551	-72.135	156.775	1.00	22.86	D	O
	ATOM	7734	N	GLY	327	6.173	-73.687	155.263	1.00	24.36	D	N
30	ATOM	7735	CA	GLY	327	7.298	-74.147	156.064	1.00	25.31	D	C
	ATOM	7736	C	GLY	327	8.252	-73.007	156.385	1.00	26.49	D	C
	ATOM	7737	O	GLY	327	8.747	-72.901	157.504	1.00	26.84	D	O
	ATOM	7738	N	TYR	328	8.518	-72.150	155.406	1.00	27.41	D	N
	ATOM	7739	CA	TYR	328	9.399	-71.006	155.623	1.00	28.77	D	C
35	ATOM	7740	CB	TYR	328	9.628	-70.263	154.306	1.00	30.90	D	C
	ATOM	7741	CG	TYR	328	10.456	-69.001	154.434	1.00	33.99	D	C
	ATOM	7742	CD1	TYR	328	11.844	-69.034	154.311	1.00	35.76	D	C
	ATOM	7743	CE1	TYR	328	12.607	-67.862	154.423	1.00	37.49	D	C
	ATOM	7744	CD2	TYR	328	9.846	-67.769	154.676	1.00	35.90	D	C
40	ATOM	7745	CE2	TYR	328	10.594	-66.594	154.793	1.00	36.85	D	C
	ATOM	7746	CZ	TYR	328	11.974	-66.645	154.664	1.00	38.17	D	C
	ATOM	7747	OH	TYR	328	12.715	-65.481	154.779	1.00	38.64	D	O
	ATOM	7748	C	TYR	328	8.768	-70.055	156.652	1.00	28.63	D	C
	ATOM	7749	O	TYR	328	9.432	-69.603	157.585	1.00	28.57	D	O
45	ATOM	7750	N	GLN	329	7.485	-69.754	156.479	1.00	27.87	D	N
	ATOM	7751	CA	GLN	329	6.781	-68.866	157.402	1.00	27.72	D	C
	ATOM	7752	CB	GLN	329	5.302	-68.747	157.005	1.00	26.32	D	C
	ATOM	7753	CG	GLN	329	5.057	-68.171	155.609	1.00	24.53	D	C
	ATOM	7754	CD	GLN	329	5.434	-66.702	155.502	1.00	24.96	D	C
50	ATOM	7755	OE1	GLN	329	6.304	-66.318	154.711	1.00	24.59	D	O
	ATOM	7756	NE2	GLN	329	4.778	-65.874	156.295	1.00	22.57	D	N
	ATOM	7757	C	GLN	329	6.881	-69.382	158.838	1.00	28.33	D	C
	ATOM	7758	O	GLN	329	7.161	-68.624	159.761	1.00	27.55	D	O
	ATOM	7759	N	ILE	330	6.659	-70.679	159.024	1.00	29.84	D	N
55	ATOM	7760	CA	ILE	330	6.705	-71.273	160.357	1.00	31.64	D	C
	ATOM	7761	CB	ILE	330	6.223	-72.744	160.324	1.00	31.62	D	C
	ATOM	7762	CG2	ILE	330	6.490	-73.431	161.668	1.00	30.48	D	C
	ATOM	7763	CG1	ILE	330	4.730	-72.787	160.000	1.00	31.78	D	C
	ATOM	7764	CD1	ILE	330	4.216	-74.195	159.714	1.00	32.07	D	C

-303-

	ATOM	7765	C	ILE	330	8.081	-71.215	161.017	1.00	33.17	D	C
	ATOM	7766	O	ILE	330	8.180	-71.044	162.233	1.00	32.52	D	O
	ATOM	7767	N	GLN	331	9.142	-71.358	160.229	1.00	34.61	D	N
5	ATOM	7768	CA	GLN	331	10.489	-71.323	160.790	1.00	36.32	D	C
	ATOM	7769	CB	GLN	331	11.462	-72.086	159.885	1.00	37.97	D	C
	ATOM	7770	CG	GLN	331	11.516	-73.581	160.175	1.00	41.59	D	C
	ATOM	7771	CD	GLN	331	11.035	-74.429	159.014	1.00	44.09	D	C
	ATOM	7772	OE1	GLN	331	11.678	-74.490	157.958	1.00	45.41	D	O
10	ATOM	7773	NE2	GLN	331	9.894	-75.091	159.201	1.00	45.77	D	N
	ATOM	7774	C	GLN	331	11.033	-69.922	161.055	1.00	36.37	D	C
	ATOM	7775	O	GLN	331	11.827	-69.732	161.973	1.00	36.85	D	O
	ATOM	7776	N	HIS	332	10.590	-68.946	160.268	1.00	36.20	D	N
	ATOM	7777	CA	HIS	332	11.060	-67.569	160.399	1.00	35.92	D	C
15	ATOM	7778	CB	HIS	332	11.273	-66.977	159.006	1.00	38.26	D	C
	ATOM	7779	CG	HIS	332	12.444	-67.562	158.281	1.00	40.86	D	C
	ATOM	7780	CD2	HIS	332	12.602	-68.754	157.656	1.00	41.83	D	C
	ATOM	7781	ND1	HIS	332	13.659	-66.916	158.186	1.00	41.67	D	N
	ATOM	7782	CE1	HIS	332	14.514	-67.684	157.535	1.00	42.92	D	C
20	ATOM	7783	NE2	HIS	332	13.899	-68.806	157.202	1.00	42.63	D	N
	ATOM	7784	C	HIS	332	10.197	-66.612	161.217	1.00	34.94	D	C
	ATOM	7785	O	HIS	332	10.631	-65.502	161.523	1.00	34.73	D	O
	ATOM	7786	N	ILE	333	8.986	-67.025	161.577	1.00	33.52	D	N
	ATOM	7787	CA	ILE	333	8.103	-66.154	162.343	1.00	31.90	D	C
25	ATOM	7788	CB	ILE	333	6.845	-65.815	161.524	1.00	32.25	D	C
	ATOM	7789	CG2	ILE	333	5.909	-64.930	162.337	1.00	31.29	D	C
	ATOM	7790	CG1	ILE	333	7.260	-65.115	160.224	1.00	31.70	D	C
	ATOM	7791	CD1	ILE	333	6.134	-64.907	159.231	1.00	31.83	D	C
	ATOM	7792	C	ILE	333	7.697	-66.776	163.670	1.00	31.12	D	C
30	ATOM	7793	O	ILE	333	6.922	-67.729	163.707	1.00	30.47	D	O
	ATOM	7794	N	GLN	334	8.230	-66.233	164.762	1.00	30.13	D	N
	ATOM	7795	CA	GLN	334	7.917	-66.747	166.092	1.00	29.64	D	C
	ATOM	7796	CB	GLN	334	8.673	-65.958	167.171	1.00	31.35	D	C
	ATOM	7797	CG	GLN	334	8.555	-66.553	168.571	1.00	35.01	D	C
35	ATOM	7798	CD	GLN	334	9.374	-65.800	169.612	1.00	38.12	D	C
	ATOM	7799	OE1	GLN	334	9.003	-64.707	170.050	1.00	39.79	D	O
	ATOM	7800	NE2	GLN	334	10.499	-66.383	170.009	1.00	40.23	D	N
	ATOM	7801	C	GLN	334	6.420	-66.670	166.366	1.00	27.88	D	C
	ATOM	7802	O	GLN	334	5.783	-65.647	166.115	1.00	25.92	D	O
40	ATOM	7803	N	GLY	335	5.861	-67.763	166.871	1.00	26.57	D	N
	ATOM	7804	CA	GLY	335	4.445	-67.785	167.186	1.00	25.42	D	C
	ATOM	7805	C	GLY	335	3.539	-68.439	166.159	1.00	23.73	D	C
	ATOM	7806	O	GLY	335	2.503	-68.977	166.525	1.00	22.96	D	O
	ATOM	7807	N	LEU	336	3.902	-68.391	164.883	1.00	23.02	D	N
45	ATOM	7808	CA	LEU	336	3.066	-69.005	163.855	1.00	23.83	D	C
	ATOM	7809	CB	LEU	336	3.673	-68.812	162.465	1.00	24.18	D	C
	ATOM	7810	CG	LEU	336	3.504	-67.489	161.718	1.00	25.08	D	C
	ATOM	7811	CD1	LEU	336	4.072	-67.659	160.312	1.00	25.55	D	C
	ATOM	7812	CD2	LEU	336	2.036	-67.096	161.640	1.00	23.47	D	C
50	ATOM	7813	C	LEU	336	2.840	-70.500	164.084	1.00	24.21	D	C
	ATOM	7814	O	LEU	336	1.755	-71.018	163.814	1.00	23.84	D	O
	ATOM	7815	N	SER	337	3.865	-71.191	164.578	1.00	24.29	D	N
	ATOM	7816	CA	SER	337	3.771	-72.624	164.827	1.00	25.75	D	C
	ATOM	7817	CB	SER	337	5.093	-73.153	165.388	1.00	26.85	D	C
	ATOM	7818	OG	SER	337	5.392	-72.529	166.625	1.00	27.91	D	O
55	ATOM	7819	C	SER	337	2.638	-72.976	165.786	1.00	25.71	D	C
	ATOM	7820	O	SER	337	2.146	-74.096	165.773	1.00	26.16	D	O
	ATOM	7821	N	ALA	338	2.232	-72.030	166.625	1.00	25.49	D	N
	ATOM	7822	CA	ALA	338	1.138	-72.272	167.556	1.00	26.59	D	C

-304-

	ATOM	7823	CB	ALA	338	0.893	-71.032	168.418	1.00	26.85	D	C
	ATOM	7824	C	ALA	338	-0.145	-72.646	166.814	1.00	27.29	D	C
	ATOM	7825	O	ALA	338	-1.029	-73.267	167.390	1.00	27.76	D	O
5	ATOM	7826	N	MET	339	-0.252	-72.262	165.545	1.00	27.52	D	N
	ATOM	7827	CA	MET	339	-1.438	-72.576	164.760	1.00	29.68	D	C
	ATOM	7828	CB	MET	339	-1.769	-71.410	163.825	1.00	26.75	D	C
	ATOM	7829	CG	MET	339	-2.256	-70.179	164.581	1.00	24.80	D	C
	ATOM	7830	SD	MET	339	-2.381	-68.721	163.556	1.00	21.82	D	S
10	ATOM	7831	CE	MET	339	-0.670	-68.330	163.361	1.00	22.13	D	C
	ATOM	7832	C	MET	339	-1.334	-73.884	163.973	1.00	32.16	D	C
	ATOM	7833	O	MET	339	-2.268	-74.263	163.271	1.00	32.08	D	O
	ATOM	7834	N	MET	340	-0.204	-74.574	164.087	1.00	36.22	D	N
	ATOM	7835	CA	MET	340	-0.037	-75.858	163.409	1.00	41.37	D	C
15	ATOM	7836	CB	MET	340	1.340	-76.439	163.713	1.00	42.92	D	C
	ATOM	7837	CG	MET	340	2.436	-75.849	162.858	1.00	45.73	D	C
	ATOM	7838	SD	MET	340	2.720	-76.818	161.366	1.00	51.37	D	S
	ATOM	7839	CE	MET	340	1.237	-76.539	160.417	1.00	49.14	D	C
	ATOM	7840	C	MET	340	-1.136	-76.798	163.904	1.00	43.73	D	C
20	ATOM	7841	O	MET	340	-1.386	-76.894	165.103	1.00	44.25	D	O
	ATOM	7842	N	PRO	341	-1.799	-77.508	162.980	1.00	46.50	D	N
	ATOM	7843	CD	PRO	341	-1.342	-77.652	161.589	1.00	47.23	D	C
	ATOM	7844	CA	PRO	341	-2.890	-78.452	163.250	1.00	49.23	D	C
	ATOM	7845	CB	PRO	341	-3.018	-79.219	161.929	1.00	48.42	D	C
25	ATOM	7846	CG	PRO	341	-1.655	-79.094	161.315	1.00	47.95	D	C
	ATOM	7847	C	PRO	341	-2.780	-79.377	164.468	1.00	51.91	D	C
	ATOM	7848	O	PRO	341	-3.065	-78.958	165.591	1.00	52.98	D	O
	ATOM	7849	N	LEU	342	-2.383	-80.630	164.255	1.00	54.46	D	N
	ATOM	7850	CA	LEU	342	-2.286	-81.583	165.360	1.00	56.95	D	C
30	ATOM	7851	CB	LEU	342	-2.563	-83.011	164.875	1.00	57.06	D	C
	ATOM	7852	CG	LEU	342	-3.860	-83.273	164.115	1.00	57.17	D	C
	ATOM	7853	CD1	LEU	342	-3.650	-82.927	162.658	1.00	57.93	D	C
	ATOM	7854	CD2	LEU	342	-4.247	-84.733	164.234	1.00	57.79	D	C
	ATOM	7855	C	LEU	342	-0.943	-81.552	166.081	1.00	58.67	D	C
35	ATOM	7856	O	LEU	342	-0.218	-82.551	166.115	1.00	58.76	D	O
	ATOM	7857	N	LEU	343	-0.619	-80.395	166.650	1.00	60.38	D	N
	ATOM	7858	CA	LEU	343	0.621	-80.224	167.391	1.00	62.04	D	C
	ATOM	7859	CB	LEU	343	0.760	-81.359	168.415	1.00	61.76	D	C
	ATOM	7860	CG	LEU	343	-0.275	-81.427	169.543	1.00	61.24	D	C
40	ATOM	7861	CD1	LEU	343	-0.183	-82.777	170.236	1.00	61.38	D	C
	ATOM	7862	CD2	LEU	343	-0.036	-80.294	170.534	1.00	61.07	D	C
	ATOM	7863	C	LEU	343	1.889	-80.121	166.534	1.00	63.41	D	C
	ATOM	7864	O	LEU	343	2.210	-79.047	166.024	1.00	63.91	D	O
	ATOM	7865	N	GLN	344	2.602	-81.234	166.373	1.00	64.75	D	N
45	ATOM	7866	CA	GLN	344	3.860	-81.256	165.616	1.00	66.45	D	C
	ATOM	7867	CB	GLN	344	4.767	-82.373	166.143	1.00	66.30	D	C
	ATOM	7868	CG	GLN	344	4.130	-83.755	166.091	1.00	65.84	D	C
	ATOM	7869	CD	GLN	344	5.143	-84.855	165.853	1.00	65.57	D	C
	ATOM	7870	OE1	GLN	344	6.097	-85.013	166.614	1.00	65.72	D	O
50	ATOM	7871	NE2	GLN	344	4.942	-85.622	164.786	1.00	65.11	D	N
	ATOM	7872	C	GLN	344	3.744	-81.414	164.104	1.00	67.47	D	C
	ATOM	7873	O	GLN	344	4.238	-82.394	163.541	1.00	67.50	D	O
	ATOM	7874	N	GLU	345	3.121	-80.446	163.441	1.00	68.16	D	N
	ATOM	7875	CA	GLU	345	2.951	-80.515	161.991	1.00	69.15	D	C
	ATOM	7876	CB	GLU	345	4.317	-80.608	161.293	1.00	69.28	D	C
55	ATOM	7877	CG	GLU	345	4.823	-79.311	160.652	1.00	69.98	D	C
	ATOM	7878	CD	GLU	345	5.541	-78.383	161.622	1.00	70.48	D	C
	ATOM	7879	OE1	GLU	345	6.710	-78.031	161.345	1.00	70.72	D	O
	ATOM	7880	OE2	GLU	345	4.944	-77.996	162.651	1.00	70.76	D	O

-305-

	ATOM	7881	C	GLU	345	2.089	-81.717	161.585	1.00	69.56	D	C
	ATOM	7882	O	GLU	345	2.212	-82.214	160.466	1.00	69.53	D	O
	ATOM	7883	N	ILE	346	1.228	-82.161	162.505	1.00	69.54	D	N
5	ATOM	7884	CA	ILE	346	0.306	-83.292	162.333	1.00	70.13	D	C
	ATOM	7885	CB	ILE	346	0.604	-84.111	161.035	1.00	69.60	D	C
	ATOM	7886	CG2	ILE	346	1.800	-85.036	161.268	1.00	69.36	D	C
	ATOM	7887	CG1	ILE	346	-0.642	-84.897	160.590	1.00	68.80	D	C
	ATOM	7888	CD1	ILE	346	-0.930	-86.167	161.379	1.00	67.66	D	C
10	ATOM	7889	C	ILE	346	0.462	-84.208	163.552	1.00	70.49	D	C
	ATOM	7890	O	ILE	346	1.504	-84.095	164.233	1.00	71.08	D	O
	ATOM	7891	OXT	ILE	346	-0.443	-85.029	163.815	1.00	71.20	D	O
	TER	7892		ILE	346							D
	ATOM	7893	O	HOH	100	1.194	-100.903	157.437	1.00	32.35	S	O
15	ATOM	7894	O	HOH	101	5.789	-101.495	107.858	1.00	41.67	S	O
	ATOM	7895	O	HOH	102	-3.286	-100.790	155.260	1.00	35.57	S	O
	ATOM	7896	O	HOH	103	-8.930	-101.202	133.287	1.00	48.12	S	O
	ATOM	7897	O	HOH	105	9.943	-103.811	110.611	1.00	44.28	S	O
	ATOM	7898	O	HOH	109	7.852	-54.504	152.498	1.00	13.54	S	O
20	ATOM	7899	O	HOH	110	1.851	-59.616	158.936	1.00	15.42	S	O
	ATOM	7900	O	HOH	111	4.061	-55.748	105.937	1.00	14.89	S	O
	ATOM	7901	O	HOH	112	-3.981	-55.392	158.482	1.00	12.72	S	O
	ATOM	7902	O	HOH	113	-8.499	-61.621	167.958	1.00	13.73	S	O
	ATOM	7903	O	HOH	114	-12.236	-61.051	158.803	1.00	15.08	S	O
25	ATOM	7904	O	HOH	115	-0.076	-79.912	152.707	1.00	21.70	S	O
	ATOM	7905	O	HOH	116	-18.234	-71.054	169.058	1.00	16.92	S	O
	ATOM	7906	O	HOH	117	8.261	-61.905	96.377	1.00	18.79	S	O
	ATOM	7907	O	HOH	118	-9.485	-73.341	172.175	1.00	20.25	S	O
	ATOM	7908	O	HOH	119	-12.684	-59.785	167.173	1.00	18.75	S	O
30	ATOM	7909	O	HOH	120	-21.219	-81.799	152.446	1.00	17.61	S	O
	ATOM	7910	O	HOH	121	-10.313	-78.143	167.136	1.00	17.35	S	O
	ATOM	7911	O	HOH	122	-0.694	-53.980	171.689	1.00	20.99	S	O
	ATOM	7912	O	HOH	123	-7.757	-54.292	111.662	1.00	17.89	S	O
	ATOM	7913	O	HOH	124	-16.140	-46.485	114.634	1.00	19.91	S	O
35	ATOM	7914	O	HOH	125	5.487	-53.523	168.579	1.00	16.20	S	O
	ATOM	7915	O	HOH	126	12.646	-74.069	123.673	1.00	19.14	S	O
	ATOM	7916	O	HOH	127	14.789	-87.134	104.722	1.00	18.59	S	O
	ATOM	7917	O	HOH	128	-1.875	-59.315	105.692	1.00	19.91	S	O
	ATOM	7918	O	HOH	129	-11.949	-41.023	122.709	1.00	19.77	S	O
40	ATOM	7919	O	HOH	130	-9.684	-54.904	96.052	1.00	20.41	S	O
	ATOM	7920	O	HOH	131	-9.323	-60.374	151.871	1.00	19.86	S	O
	ATOM	7921	O	HOH	132	-11.101	-60.624	169.075	1.00	18.09	S	O
	ATOM	7922	O	HOH	133	-16.739	-45.232	95.584	1.00	22.60	S	O
	ATOM	7923	O	HOH	134	18.286	-72.825	104.279	1.00	20.39	S	O
45	ATOM	7924	O	HOH	135	-4.303	-46.906	168.333	1.00	22.87	S	O
	ATOM	7925	O	HOH	137	-10.988	-71.168	169.786	1.00	25.18	S	O
	ATOM	7926	O	HOH	138	-9.260	-59.172	170.779	1.00	18.48	S	O
	ATOM	7927	O	HOH	139	17.621	-68.755	116.205	1.00	18.82	S	O
	ATOM	7928	O	HOH	140	-1.448	-79.558	111.697	1.00	22.23	S	O
	ATOM	7929	O	HOH	141	-18.854	-71.097	159.796	1.00	19.71	S	O
50	ATOM	7930	O	HOH	142	-5.714	-58.929	112.169	1.00	20.72	S	O
	ATOM	7931	O	HOH	143	-7.023	-46.850	93.588	1.00	25.75	S	O
	ATOM	7932	O	HOH	144	16.216	-32.288	156.566	1.00	21.61	S	O
	ATOM	7933	O	HOH	145	-9.388	-44.992	163.145	1.00	18.35	S	O
	ATOM	7934	O	HOH	146	-13.382	-72.973	140.426	1.00	21.72	S	O
55	ATOM	7935	O	HOH	147	12.712	-41.533	141.695	1.00	18.66	S	O
	ATOM	7936	O	HOH	148	-15.805	-42.708	103.032	1.00	16.53	S	O
	ATOM	7937	O	HOH	149	19.880	-87.184	117.113	1.00	23.48	S	O
	ATOM	7938	O	HOH	150	16.442	-43.255	161.564	1.00	25.71	S	O

-306-

5	ATOM	7939	O	HOH	151	-5.245	-53.158	95.611	1.00	17.95	S	O
	ATOM	7940	O	HOH	152	5.815	-59.391	152.298	1.00	19.34	S	O
	ATOM	7941	O	HOH	153	6.055	-55.938	171.262	1.00	19.01	S	O
	ATOM	7942	O	HOH	154	9.371	-61.052	112.669	1.00	19.61	S	O
	ATOM	7943	O	HOH	155	-2.818	-61.077	171.684	1.00	18.36	S	O
10	ATOM	7944	O	HOH	156	7.580	-55.929	112.685	1.00	20.71	S	O
	ATOM	7945	O	HOH	157	-1.829	-35.248	152.635	1.00	21.17	S	O
	ATOM	7946	O	HOH	158	-12.998	-38.744	111.352	1.00	22.19	S	O
	ATOM	7947	O	HOH	159	-10.033	-57.313	153.074	1.00	26.61	S	O
	ATOM	7948	O	HOH	160	-14.613	-42.493	121.850	1.00	21.46	S	O
15	ATOM	7949	O	HOH	161	-0.465	-59.730	96.207	1.00	22.15	S	O
	ATOM	7950	O	HOH	162	-1.457	-79.928	119.289	1.00	25.62	S	O
	ATOM	7951	O	HOH	163	-2.242	-34.614	155.101	1.00	24.72	S	O
	ATOM	7952	O	HOH	164	-2.488	-28.817	149.752	1.00	24.52	S	O
	ATOM	7953	O	HOH	165	-14.811	-78.255	132.956	1.00	26.75	S	O
20	ATOM	7954	O	HOH	166	8.396	-73.450	91.962	1.00	24.27	S	O
	ATOM	7955	O	HOH	167	2.582	-61.210	92.554	1.00	19.81	S	O
	ATOM	7956	O	HOH	168	0.065	-36.237	163.877	1.00	22.12	S	O
	ATOM	7957	O	HOH	169	9.793	-55.410	168.376	1.00	22.34	S	O
	ATOM	7958	O	HOH	170	-8.169	-68.504	136.548	1.00	25.65	S	O
25	ATOM	7959	O	HOH	171	-7.200	-55.767	151.754	1.00	21.47	S	O
	ATOM	7960	O	HOH	172	-12.681	-37.331	109.182	1.00	20.87	S	O
	ATOM	7961	O	HOH	173	16.665	-83.359	109.157	1.00	22.25	S	O
	ATOM	7962	O	HOH	174	8.904	-17.589	154.270	1.00	32.11	S	O
	ATOM	7963	O	HOH	175	-9.871	-57.482	160.770	1.00	22.21	S	O
30	ATOM	7964	O	HOH	176	10.054	-68.265	94.306	1.00	22.03	S	O
	ATOM	7965	O	HOH	177	-7.645	-35.523	134.429	1.00	33.35	S	O
	ATOM	7966	O	HOH	178	-17.960	-31.774	109.544	1.00	26.39	S	O
	ATOM	7967	O	HOH	179	2.162	-42.472	136.264	1.00	25.98	S	O
	ATOM	7968	O	HOH	180	3.481	-55.715	96.425	1.00	21.71	S	O
35	ATOM	7969	O	HOH	181	-1.946	-59.108	170.157	1.00	21.79	S	O
	ATOM	7970	O	HOH	182	0.579	-86.300	149.857	1.00	29.11	S	O
	ATOM	7971	O	HOH	183	-7.526	-45.845	127.493	1.00	22.42	S	O
	ATOM	7972	O	HOH	184	-17.611	-43.737	111.356	1.00	24.87	S	O
	ATOM	7973	O	HOH	185	-7.509	-69.242	100.449	1.00	23.13	S	O
40	ATOM	7974	O	HOH	186	-5.332	-93.514	158.577	1.00	22.53	S	O
	ATOM	7975	O	HOH	187	10.436	-93.075	106.554	1.00	23.92	S	O
	ATOM	7976	O	HOH	188	9.310	-52.599	171.929	1.00	27.84	S	O
	ATOM	7977	O	HOH	189	16.827	-47.166	149.767	1.00	22.64	S	O
	ATOM	7978	O	HOH	190	2.500	-15.666	156.796	1.00	24.25	S	O
45	ATOM	7979	O	HOH	191	0.395	-59.578	168.198	1.00	26.75	S	O
	ATOM	7980	O	HOH	192	8.107	-33.555	114.378	1.00	28.48	S	O
	ATOM	7981	O	HOH	193	-7.319	-49.935	168.792	1.00	27.62	S	O
	ATOM	7982	O	HOH	194	-8.208	-31.818	100.278	1.00	23.15	S	O
	ATOM	7983	O	HOH	195	7.764	-47.435	170.758	1.00	21.29	S	O
50	ATOM	7984	O	HOH	196	7.480	-88.122	101.942	1.00	26.44	S	O
	ATOM	7985	O	HOH	197	14.406	-62.102	94.383	1.00	23.98	S	O
	ATOM	7986	O	HOH	198	-15.741	-40.088	122.107	1.00	26.12	S	O
	ATOM	7987	O	HOH	199	-1.448	-56.070	170.098	1.00	28.03	S	O
	ATOM	7988	O	HOH	200	5.541	-47.303	95.880	1.00	28.11	S	O
55	ATOM	7989	O	HOH	201	-12.575	-56.737	102.862	1.00	31.08	S	O
	ATOM	7990	O	HOH	202	1.715	-58.973	94.236	1.00	25.62	S	O
	ATOM	7991	O	HOH	203	9.480	-63.602	164.661	1.00	25.82	S	O
	ATOM	7992	O	HOH	204	-1.232	-35.010	144.845	1.00	24.54	S	O
	ATOM	7993	O	HOH	205	7.562	-71.697	147.929	1.00	26.32	S	O
	ATOM	7994	O	HOH	207	-7.835	-53.973	94.498	1.00	22.20	S	O
	ATOM	7995	O	HOH	208	7.846	-54.379	169.964	1.00	24.84	S	O
	ATOM	7996	O	HOH	209	2.796	-35.267	111.786	1.00	27.64	S	O

-307-

	ATOM	7997	O	HOH	210	4.203	-78.801	135.459	1.00	24.54	S	O
	ATOM	7998	O	HOH	211	-18.964	-44.018	109.109	1.00	21.20	S	O
	ATOM	7999	O	HOH	212	-17.685	-49.045	107.242	1.00	27.48	S	O
5	ATOM	8000	O	HOH	213	19.295	-89.525	117.193	1.00	28.97	S	O
	ATOM	8001	O	HOH	214	9.997	-58.041	111.888	1.00	34.69	S	O
	ATOM	8002	O	HOH	215	-15.068	-31.753	107.636	1.00	27.99	S	O
	ATOM	8003	O	HOH	216	-18.184	-67.421	148.176	1.00	20.26	S	O
	ATOM	8004	O	HOH	217	-5.170	-78.598	128.888	1.00	25.97	S	O
10	ATOM	8005	O	HOH	218	8.686	-78.683	97.186	1.00	27.25	S	O
	ATOM	8006	O	HOH	219	7.141	-79.540	135.217	1.00	21.04	S	O
	ATOM	8007	O	HOH	220	8.066	-46.341	137.131	1.00	21.84	S	O
	ATOM	8008	O	HOH	221	-0.483	-13.878	155.199	1.00	29.72	S	O
	ATOM	8009	O	HOH	222	9.453	-32.021	164.111	1.00	23.90	S	O
	ATOM	8010	O	HOH	223	11.544	-18.447	160.393	1.00	21.15	S	O
15	ATOM	8011	O	HOH	224	-6.546	-76.779	168.538	1.00	23.30	S	O
	ATOM	8012	O	HOH	225	-10.762	-67.817	169.854	1.00	25.60	S	O
	ATOM	8013	O	HOH	226	-8.111	-57.123	110.725	1.00	25.49	S	O
	ATOM	8014	O	HOH	227	-23.033	-74.790	169.157	1.00	27.54	S	O
	ATOM	8015	O	HOH	228	-14.901	-61.518	170.186	1.00	26.01	S	O
20	ATOM	8016	O	HOH	229	-12.533	-51.396	163.830	1.00	24.68	S	O
	ATOM	8017	O	HOH	230	-7.243	-33.221	149.831	1.00	27.89	S	O
	ATOM	8018	O	HOH	231	9.051	-59.422	93.575	1.00	25.99	S	O
	ATOM	8019	O	HOH	232	-1.525	-42.199	127.967	1.00	28.31	S	O
	ATOM	8020	O	HOH	233	-6.126	-55.469	92.922	1.00	24.15	S	O
25	ATOM	8021	O	HOH	234	10.308	-22.755	159.042	1.00	24.72	S	O
	ATOM	8022	O	HOH	235	-11.576	-58.094	151.433	1.00	35.81	S	O
	ATOM	8023	O	HOH	236	-10.101	-53.349	104.435	1.00	29.28	S	O
	ATOM	8024	O	HOH	237	12.619	-60.351	97.081	1.00	22.39	S	O
	ATOM	8025	O	HOH	238	15.329	-43.209	142.529	1.00	25.98	S	O
30	ATOM	8026	O	HOH	239	1.005	-54.014	92.643	1.00	28.69	S	O
	ATOM	8027	O	HOH	240	14.968	-36.448	134.614	1.00	27.47	S	O
	ATOM	8028	O	HOH	241	7.889	-69.278	128.039	1.00	25.45	S	O
	ATOM	8029	O	HOH	242	1.344	-56.173	94.149	1.00	25.84	S	O
	ATOM	8030	O	HOH	243	-13.791	-43.127	93.512	1.00	31.21	S	O
35	ATOM	8031	O	HOH	244	11.904	-53.435	171.337	1.00	24.49	S	O
	ATOM	8032	O	HOH	245	6.729	-70.309	164.313	1.00	26.33	S	O
	ATOM	8033	O	HOH	246	11.002	-83.852	100.804	1.00	35.04	S	O
	ATOM	8034	O	HOH	247	15.286	-72.468	123.050	1.00	27.65	S	O
	ATOM	8035	O	HOH	248	-0.135	-80.031	144.939	1.00	33.14	S	O
40	ATOM	8036	O	HOH	249	-12.834	-28.015	103.311	1.00	25.83	S	O
	ATOM	8037	O	HOH	250	-22.846	-93.032	149.641	1.00	32.57	S	O
	ATOM	8038	O	HOH	251	-7.573	-29.078	153.382	1.00	27.18	S	O
	ATOM	8039	O	HOH	252	-7.351	-48.624	149.250	1.00	26.80	S	O
	ATOM	8040	O	HOH	253	-2.336	-85.962	114.494	1.00	26.39	S	O
45	ATOM	8041	O	HOH	254	0.278	-63.451	89.646	1.00	30.34	S	O
	ATOM	8042	O	HOH	255	-20.535	-65.003	155.492	1.00	32.02	S	O
	ATOM	8043	O	HOH	256	-22.578	-25.815	109.375	1.00	28.54	S	O
	ATOM	8044	O	HOH	257	18.028	-44.064	153.151	1.00	29.77	S	O
	ATOM	8045	O	HOH	258	-16.929	-65.999	143.846	1.00	33.05	S	O
50	ATOM	8046	O	HOH	259	-16.652	-93.009	149.403	1.00	23.81	S	O
	ATOM	8047	O	HOH	260	5.808	-55.573	161.866	1.00	27.32	S	O
	ATOM	8048	O	HOH	261	-18.479	-82.008	154.705	1.00	26.16	S	O
	ATOM	8049	O	HOH	263	7.113	-14.552	156.022	1.00	33.90	S	O
	ATOM	8050	O	HOH	264	16.364	-48.844	145.484	1.00	31.20	S	O
55	ATOM	8051	O	HOH	265	1.628	-80.074	138.485	1.00	27.26	S	O
	ATOM	8052	O	HOH	266	5.293	-76.738	95.657	1.00	30.99	S	O
	ATOM	8053	O	HOH	267	7.573	-60.159	114.770	1.00	31.64	S	O
	ATOM	8054	O	HOH	268	14.544	-43.496	170.824	1.00	25.33	S	O

-308-

5	ATOM	8055	O	HOH	269	-10.804	-71.018	173.076	1.00	32.63	S	O
	ATOM	8056	O	HOH	270	3.311	-62.924	146.402	1.00	29.18	S	O
	ATOM	8057	O	HOH	271	5.357	-53.638	90.691	1.00	31.79	S	O
	ATOM	8058	O	HOH	272	5.227	-86.281	154.159	1.00	31.53	S	O
	ATOM	8059	O	HOH	273	9.855	-19.105	158.633	1.00	29.74	S	O
10	ATOM	8060	O	HOH	274	-20.468	-80.759	149.925	1.00	33.49	S	O
	ATOM	8061	O	HOH	275	-5.662	-97.233	157.623	1.00	30.30	S	O
	ATOM	8062	O	HOH	276	15.625	-37.089	150.881	1.00	35.21	S	O
	ATOM	8063	O	HOH	277	12.161	-61.189	105.768	1.00	33.96	S	O
	ATOM	8064	O	HOH	278	3.234	-34.573	109.191	1.00	33.68	S	O
15	ATOM	8065	O	HOH	279	-8.880	-47.618	151.419	1.00	28.74	S	O
	ATOM	8066	O	HOH	280	-22.502	-91.753	152.263	1.00	27.73	S	O
	ATOM	8067	O	HOH	281	9.619	-44.170	117.572	1.00	31.74	S	O
	ATOM	8068	O	HOH	282	-15.815	-48.188	119.110	1.00	31.25	S	O
	ATOM	8069	O	HOH	283	19.218	-87.258	107.333	1.00	29.49	S	O
20	ATOM	8070	O	HOH	284	-7.873	-59.325	161.206	1.00	27.49	S	O
	ATOM	8071	O	HOH	285	10.850	-61.174	95.346	1.00	25.49	S	O
	ATOM	8072	O	HOH	286	-9.010	-43.808	146.840	1.00	28.55	S	O
	ATOM	8073	O	HOH	287	6.572	-57.925	161.333	1.00	30.97	S	O
	ATOM	8074	O	HOH	288	-8.215	-58.208	107.050	1.00	31.85	S	O
25	ATOM	8075	O	HOH	289	3.955	-65.295	169.467	1.00	31.60	S	O
	ATOM	8076	O	HOH	290	-14.833	-96.003	155.699	1.00	35.00	S	O
	ATOM	8077	O	HOH	291	7.343	-67.777	152.640	1.00	28.95	S	O
	ATOM	8078	O	HOH	292	3.887	-59.382	160.774	1.00	34.06	S	O
	ATOM	8079	O	HOH	293	-17.158	-41.652	112.721	1.00	25.07	S	O
30	ATOM	8080	O	HOH	294	14.325	-28.388	160.924	1.00	37.13	S	O
	ATOM	8081	O	HOH	295	9.748	-49.591	171.437	1.00	31.26	S	O
	ATOM	8082	O	HOH	296	-8.483	-70.123	175.216	1.00	31.58	S	O
	ATOM	8083	O	HOH	297	-3.228	-55.653	168.111	1.00	25.65	S	O
	ATOM	8084	O	HOH	298	1.280	-57.553	99.814	1.00	35.96	S	O
35	ATOM	8085	O	HOH	299	1.782	-67.747	169.041	1.00	27.46	S	O
	ATOM	8086	O	HOH	300	19.076	-71.750	112.954	1.00	31.18	S	O
	ATOM	8087	O	HOH	301	7.766	-50.185	95.554	1.00	35.30	S	O
	ATOM	8088	O	HOH	302	-19.172	-73.024	170.669	1.00	28.28	S	O
	ATOM	8089	O	HOH	303	6.550	-66.338	127.917	1.00	33.15	S	O
40	ATOM	8090	O	HOH	304	-7.882	-67.023	112.124	1.00	35.97	S	O
	ATOM	8091	O	HOH	305	3.276	-41.817	170.536	1.00	26.99	S	O
	ATOM	8092	O	HOH	306	-10.797	-27.751	98.382	1.00	29.26	S	O
	ATOM	8093	O	HOH	307	10.141	-71.189	94.544	1.00	41.52	S	O
	ATOM	8094	O	HOH	308	-2.498	-17.923	102.659	1.00	41.26	S	O
45	ATOM	8095	O	HOH	309	6.943	-48.634	136.885	1.00	30.49	S	O
	ATOM	8096	O	HOH	310	17.016	-82.948	106.465	1.00	34.52	S	O
	ATOM	8097	O	HOH	311	9.961	-31.840	166.802	1.00	25.52	S	O
	ATOM	8098	O	HOH	312	16.318	-75.014	123.176	1.00	29.99	S	O
	ATOM	8099	O	HOH	313	-8.320	-78.457	169.043	1.00	27.78	S	O
50	ATOM	8100	O	HOH	314	-3.295	-62.615	118.169	1.00	39.70	S	O
	ATOM	8101	O	HOH	315	-9.600	-68.541	177.428	1.00	40.70	S	O
	ATOM	8102	O	HOH	316	18.848	-24.865	153.276	1.00	26.59	S	O
	ATOM	8103	O	HOH	317	18.065	-41.975	151.565	1.00	30.90	S	O
	ATOM	8104	O	HOH	318	-7.505	-17.390	109.924	1.00	35.70	S	O
55	ATOM	8105	O	HOH	319	-13.354	-57.093	167.637	1.00	27.84	S	O
	ATOM	8106	O	HOH	320	-15.940	-71.333	141.033	1.00	34.15	S	O
	ATOM	8107	O	HOH	321	-14.330	-37.004	129.073	1.00	35.91	S	O
	ATOM	8108	O	HOH	323	5.371	-37.013	108.859	1.00	40.25	S	O
	ATOM	8109	O	HOH	324	8.427	-57.724	153.806	1.00	29.58	S	O
55	ATOM	8110	O	HOH	325	-15.957	-77.661	148.698	1.00	38.84	S	O
	ATOM	8111	O	HOH	326	-19.744	-69.811	151.149	1.00	33.24	S	O
	ATOM	8112	O	HOH	327	13.585	-37.762	154.701	1.00	36.77	S	O

-309-

5	ATOM	8113	O	HOH	328	-4.082	-52.659	145.859	1.00	35.37	S	O
	ATOM	8114	O	HOH	329	-12.214	-97.380	152.729	1.00	40.91	S	O
	ATOM	8115	O	HOH	330	21.253	-78.801	100.196	1.00	41.54	S	O
	ATOM	8116	O	HOH	331	20.349	-66.162	108.672	1.00	39.01	S	O
	ATOM	8117	O	HOH	332	14.913	-47.738	137.531	1.00	41.04	S	O
	ATOM	8118	O	HOH	333	4.138	-44.506	175.935	1.00	34.58	S	O
	ATOM	8119	O	HOH	334	-23.111	-25.163	112.021	1.00	44.12	S	O
10	ATOM	8120	O	HOH	335	14.393	-21.278	151.249	1.00	38.52	S	O
	ATOM	8121	O	HOH	336	-7.214	-56.582	102.979	1.00	30.20	S	O
	ATOM	8122	O	HOH	337	-10.229	-62.939	99.872	1.00	30.38	S	O
	ATOM	8123	O	HOH	338	19.511	-44.397	155.298	1.00	29.41	S	O
15	ATOM	8124	O	HOH	339	22.143	-74.211	95.233	1.00	32.45	S	O
	ATOM	8125	O	HOH	340	-3.916	-30.077	164.362	1.00	31.78	S	O
	ATOM	8126	O	HOH	341	19.294	-80.459	105.562	1.00	28.04	S	O
	ATOM	8127	O	HOH	343	-14.436	-22.122	109.753	1.00	42.19	S	O
	ATOM	8128	O	HOH	344	-18.980	-68.857	170.396	1.00	27.91	S	O
20	ATOM	8129	O	HOH	345	14.112	-22.558	160.678	1.00	43.95	S	O
	ATOM	8130	O	HOH	346	18.274	-93.064	117.144	1.00	35.29	S	O
	ATOM	8131	O	HOH	347	-8.246	-70.761	116.848	1.00	34.25	S	O
	ATOM	8132	O	HOH	348	-18.491	-45.415	113.302	1.00	34.77	S	O
	ATOM	8133	O	HOH	349	-23.016	-83.847	145.069	1.00	31.88	S	O
	ATOM	8134	O	HOH	350	10.529	-57.869	168.903	1.00	37.36	S	O
25	ATOM	8135	O	HOH	351	-11.064	-99.719	153.017	1.00	32.52	S	O
	ATOM	8136	O	HOH	352	-18.605	-57.435	156.021	1.00	48.54	S	O
	ATOM	8137	O	HOH	353	6.820	-51.420	145.123	1.00	26.19	S	O
	ATOM	8138	O	HOH	354	7.424	-70.606	166.993	1.00	42.35	S	O
	ATOM	8139	O	HOH	355	-21.257	-69.634	153.100	1.00	30.60	S	O
30	ATOM	8140	O	HOH	356	-5.428	-53.184	173.508	1.00	47.01	S	O
	ATOM	8141	O	HOH	358	1.762	-72.692	128.237	1.00	31.19	S	O
	ATOM	8142	O	HOH	359	-10.579	-56.732	156.601	1.00	29.22	S	O
	ATOM	8143	O	HOH	360	10.074	-45.397	100.980	1.00	27.83	S	O
	ATOM	8144	O	HOH	361	-5.271	-36.663	96.236	1.00	37.52	S	O
35	ATOM	8145	O	HOH	362	16.417	-35.156	149.391	1.00	39.87	S	O
	ATOM	8146	O	HOH	363	-19.386	-54.167	164.566	1.00	29.90	S	O
	ATOM	8147	O	HOH	364	10.075	-46.599	135.114	1.00	32.66	S	O
	ATOM	8148	O	HOH	365	-14.091	-91.529	157.785	1.00	32.62	S	O
	ATOM	8149	O	HOH	366	-20.701	-38.092	109.527	1.00	39.14	S	O
40	ATOM	8150	O	HOH	367	-7.386	-93.366	159.935	1.00	30.91	S	O
	ATOM	8151	O	HOH	369	-16.339	-34.495	103.921	1.00	33.02	S	O
	ATOM	8152	O	HOH	370	-2.829	-44.378	128.744	1.00	35.96	S	O
	ATOM	8153	O	HOH	371	17.549	-68.539	122.607	1.00	39.74	S	O
	ATOM	8154	O	HOH	372	-3.480	-70.209	170.898	1.00	33.17	S	O
45	ATOM	8155	O	HOH	373	-11.040	-39.910	157.889	1.00	47.16	S	O
	ATOM	8156	O	HOH	374	7.105	-47.482	173.306	1.00	31.81	S	O
	ATOM	8157	O	HOH	375	-18.558	-91.764	156.839	1.00	43.43	S	O
	ATOM	8158	O	HOH	376	14.500	-36.034	147.266	1.00	33.03	S	O
	ATOM	8159	O	HOH	377	5.441	-13.946	152.019	1.00	31.07	S	O
50	ATOM	8160	O	HOH	378	-15.436	-76.101	134.105	1.00	37.41	S	O
	ATOM	8161	O	HOH	379	-11.954	-99.496	157.807	1.00	44.33	S	O
	ATOM	8162	O	HOH	380	-6.554	-48.748	127.555	1.00	35.49	S	O
	ATOM	8163	O	HOH	381	-8.509	-66.978	173.073	1.00	35.86	S	O
	ATOM	8164	O	HOH	383	17.282	-95.348	108.536	1.00	37.37	S	O
55	ATOM	8165	O	HOH	385	3.084	-70.354	129.029	1.00	41.45	S	O
	ATOM	8166	O	HOH	386	-8.676	-18.921	105.307	1.00	44.00	S	O
	ATOM	8167	O	HOH	387	21.378	-36.435	164.207	1.00	37.54	S	O
	ATOM	8168	O	HOH	388	9.895	-68.660	130.123	1.00	34.65	S	O
	ATOM	8169	O	HOH	389	13.876	-94.055	114.570	1.00	35.97	S	O
	ATOM	8170	O	HOH	390	-2.415	-72.576	135.885	1.00	30.52	S	O

-310-

	ATOM	8171	O	HOH	391	-8.453	-70.094	98.112	1.00	40.15	S	O
	ATOM	8172	O	HOH	392	-4.178	-80.568	127.822	1.00	31.47	S	O
	ATOM	8173	O	HOH	393	-17.842	-63.215	143.635	1.00	39.38	S	O
5	ATOM	8174	O	HOH	394	-19.264	-81.648	157.206	1.00	32.27	S	O
	ATOM	8175	O	HOH	396	-20.956	-75.317	171.042	1.00	33.04	S	O
	ATOM	8176	O	HOH	397	1.082	-45.036	161.177	1.00	36.77	S	O
	ATOM	8177	O	HOH	399	-16.486	-93.083	157.191	1.00	38.04	S	O
	ATOM	8178	O	HOH	400	18.520	-69.299	94.579	1.00	38.46	S	O
10	ATOM	8179	O	HOH	401	-14.376	-47.406	162.731	1.00	43.61	S	O
	ATOM	8180	O	HOH	402	-15.725	-46.681	93.561	1.00	36.70	S	O
	ATOM	8181	O	HOH	403	15.449	-93.447	107.056	1.00	42.96	S	O
	ATOM	8182	O	HOH	404	17.756	-34.951	160.597	1.00	38.74	S	O
	ATOM	8183	O	HOH	405	-11.516	-52.980	92.984	1.00	31.69	S	O
15	ATOM	8184	O	HOH	406	2.904	-99.028	157.874	1.00	35.56	S	O
	ATOM	8185	O	HOH	407	3.990	-47.232	174.280	1.00	54.42	S	O
	ATOM	8186	O	HOH	408	5.363	-82.052	150.581	1.00	39.03	S	O
	ATOM	8187	O	HOH	409	-13.329	-21.194	112.697	1.00	38.48	S	O
	ATOM	8188	O	HOH	410	-20.132	-46.572	109.024	1.00	42.34	S	O
20	ATOM	8189	O	HOH	411	-20.146	-71.594	142.398	1.00	48.84	S	O
	ATOM	8190	O	HOH	413	7.810	-96.588	117.307	1.00	48.54	S	O
	ATOM	8191	O	HOH	414	-15.707	-39.444	112.856	1.00	30.16	S	O
	ATOM	8192	O	HOH	415	-7.705	-43.981	141.677	1.00	42.54	S	O
	ATOM	8193	O	HOH	416	-11.327	-80.716	166.581	1.00	29.92	S	O
25	ATOM	8194	O	HOH	417	14.765	-15.174	132.791	1.00	46.34	S	O
	ATOM	8195	O	HOH	418	12.180	-35.626	148.220	1.00	43.95	S	O
	ATOM	8196	O	HOH	419	-0.687	-69.344	171.152	1.00	37.41	S	O
	ATOM	8197	O	HOH	420	-11.442	-58.044	158.798	1.00	36.92	S	O
	ATOM	8198	O	HOH	421	12.102	-62.691	93.583	1.00	34.13	S	O
30	ATOM	8199	O	HOH	422	-3.773	-38.085	92.262	1.00	52.29	S	O
	ATOM	8200	O	HOH	423	12.749	-96.511	113.885	1.00	39.83	S	O
	ATOM	8201	O	HOH	424	2.752	-31.848	124.578	1.00	44.26	S	O
	ATOM	8202	O	HOH	425	12.704	-41.353	112.133	1.00	44.28	S	O
	ATOM	8203	O	HOH	427	-10.440	-68.616	172.311	1.00	32.78	S	O
35	ATOM	8204	O	HOH	428	-6.952	-47.164	90.926	1.00	36.61	S	O
	ATOM	8205	O	HOH	429	-5.052	-57.339	148.491	1.00	39.32	S	O
	ATOM	8206	O	HOH	431	-1.897	-61.286	90.062	1.00	52.91	S	O
	ATOM	8207	O	HOH	432	17.295	-72.124	95.247	1.00	51.20	S	O
	ATOM	8208	O	HOH	433	-8.442	-44.268	167.166	1.00	38.87	S	O
40	ATOM	8209	O	HOH	434	17.130	-51.752	145.075	1.00	37.31	S	O
	ATOM	8210	O	HOH	435	-11.934	-41.853	89.278	1.00	35.15	S	O
	ATOM	8211	O	HOH	436	-20.655	-79.110	158.422	1.00	38.37	S	O
	ATOM	8212	O	HOH	437	-17.692	-58.619	152.324	1.00	39.50	S	O
	ATOM	8213	O	HOH	438	-13.228	-92.072	160.458	1.00	42.10	S	O
45	ATOM	8214	O	HOH	439	4.172	-12.941	153.839	1.00	33.74	S	O
	ATOM	8215	O	HOH	440	-10.145	-87.720	162.303	1.00	38.35	S	O
	ATOM	8216	O	HOH	442	-10.931	-61.150	93.207	1.00	45.01	S	O
	ATOM	8217	O	HOH	443	-1.358	-40.495	93.770	1.00	37.78	S	O
	ATOM	8218	O	HOH	446	-6.450	-68.499	173.937	1.00	37.62	S	O
50	ATOM	8219	O	HOH	448	24.212	-70.506	107.734	1.00	48.81	S	O
	ATOM	8220	O	HOH	449	-6.596	-43.865	93.009	1.00	32.44	S	O
	ATOM	8221	O	HOH	450	-7.000	-38.908	142.094	1.00	43.17	S	O
	ATOM	8222	O	HOH	452	11.741	-63.298	155.435	1.00	33.39	S	O
	ATOM	8223	O	HOH	453	-4.596	-14.237	111.600	1.00	45.05	S	O
55	ATOM	8224	O	HOH	454	16.341	-40.682	142.327	1.00	37.42	S	O
	ATOM	8225	O	HOH	455	1.573	-61.767	174.211	1.00	40.92	S	O
	ATOM	8226	O	HOH	456	-13.624	-35.519	117.025	1.00	35.47	S	O
	ATOM	8227	O	HOH	458	-16.126	-56.335	151.820	1.00	35.23	S	O
	ATOM	8228	O	HOH	459	17.663	-37.767	143.893	1.00	40.21	S	O

-311-

	ATOM	8229	O	HOH	461	-12.126	-88.570	116.265	1.00	53.95	S	O
	ATOM	8230	O	HOH	462	1.237	-12.385	154.041	1.00	34.36	S	O
	ATOM	8231	O	HOH	463	6.955	-61.641	124.334	1.00	42.87	S	O
	ATOM	8232	O	HOH	464	3.802	-88.839	136.236	1.00	51.28	S	O
5	ATOM	8233	O	HOH	465	-1.268	-57.821	164.497	1.00	39.77	S	O
	ATOM	8234	O	HOH	466	0.366	-70.873	125.729	1.00	43.43	S	O
	ATOM	8235	O	HOH	467	2.705	-61.794	90.011	1.00	43.72	S	O
	ATOM	8236	O	HOH	468	3.798	-18.321	160.863	1.00	44.03	S	O
10	ATOM	8237	O	HOH	469	2.275	-34.938	119.431	1.00	37.93	S	O
	ATOM	8238	O	HOH	470	-3.650	-77.137	108.828	1.00	47.92	S	O
	ATOM	8239	O	HOH	472	-4.726	-64.694	95.196	1.00	35.25	S	O
	ATOM	8240	O	HOH	473	-22.754	-72.240	159.906	1.00	34.93	S	O
	ATOM	8241	O	HOH	474	16.681	-66.920	120.698	1.00	34.05	S	O
	ATOM	8242	O	HOH	475	-10.065	-60.263	173.767	1.00	42.11	S	O
15	ATOM	8243	O	HOH	476	-6.797	-14.864	110.275	1.00	38.54	S	O
	ATOM	8244	O	HOH	477	16.699	-92.866	125.208	1.00	39.15	S	O
	ATOM	8245	O	HOH	478	-8.371	-55.088	161.316	1.00	43.44	S	O
	ATOM	8246	O	HOH	479	-10.360	-72.131	177.271	1.00	57.30	S	O
20	ATOM	8247	O	HOH	481	-10.827	-16.909	116.124	1.00	45.61	S	O
	ATOM	8248	O	HOH	483	3.497	-28.876	114.517	1.00	38.30	S	O
	ATOM	8249	O	HOH	485	16.708	-79.915	98.646	1.00	36.18	S	O
	ATOM	8250	O	HOH	486	5.685	-70.865	142.719	1.00	39.47	S	O
	ATOM	8251	O	HOH	487	6.377	-57.579	115.024	1.00	44.49	S	O
	ATOM	8252	O	HOH	489	8.085	-58.272	171.632	1.00	41.31	S	O
25	ATOM	8253	O	HOH	490	-23.161	-75.958	161.598	1.00	53.30	S	O
	ATOM	8254	O	HOH	491	5.795	-69.729	129.532	1.00	41.18	S	O
	ATOM	8255	O	HOH	492	5.900	-77.072	154.533	1.00	36.96	S	O
	ATOM	8256	O	HOH	493	9.143	-81.316	97.155	1.00	35.88	S	O
	ATOM	8257	O	HOH	494	-18.609	-33.852	121.694	1.00	33.42	S	O
30	ATOM	8258	O	HOH	495	9.282	-47.550	112.568	1.00	35.91	S	O
	ATOM	8259	O	HOH	496	13.335	-57.030	154.593	1.00	47.05	S	O
	ATOM	8260	O	HOH	497	19.590	-25.131	148.612	1.00	39.22	S	O
	ATOM	8261	O	HOH	498	-10.245	-19.394	103.261	1.00	39.63	S	O
	ATOM	8262	O	HOH	499	-14.636	-36.366	113.518	1.00	34.44	S	O
35	ATOM	8263	O	HOH	500	-11.669	-46.517	135.894	1.00	47.58	S	O
	ATOM	8264	O	HOH	501	11.046	-44.408	115.223	1.00	39.61	S	O
	ATOM	8265	O	HOH	502	8.924	-97.965	124.095	1.00	51.93	S	O
	ATOM	8266	O	HOH	503	-20.620	-79.729	140.453	1.00	46.40	S	O
	ATOM	8267	O	HOH	504	-1.452	-14.657	134.440	1.00	46.55	S	O
40	ATOM	8268	O	HOH	505	9.863	-68.377	91.670	1.00	46.90	S	O
	ATOM	8269	O	HOH	506	-19.111	-50.747	108.740	1.00	42.45	S	O
	ATOM	8270	O	HOH	508	-23.485	-75.343	153.730	1.00	42.69	S	O
	ATOM	8271	O	HOH	509	-22.791	-46.334	107.564	1.00	43.38	S	O
	ATOM	8272	O	HOH	510	-18.626	-49.390	155.934	1.00	48.47	S	O
45	ATOM	8273	O	HOH	511	15.489	-38.374	135.988	1.00	43.55	S	O
	ATOM	8274	O	HOH	512	16.473	-78.340	114.704	1.00	39.28	S	O
	ATOM	8275	O	HOH	513	8.336	-58.164	157.603	1.00	42.13	S	O
	ATOM	8276	O	HOH	514	6.254	-67.387	143.859	1.00	48.19	S	O
	ATOM	8277	O	HOH	515	-9.807	-68.109	113.699	1.00	41.10	S	O
50	ATOM	8278	O	HOH	516	-16.817	-83.940	162.242	1.00	53.03	S	O
	ATOM	8279	O	HOH	517	2.380	-62.048	120.083	1.00	50.51	S	O
	ATOM	8280	O	HOH	518	-7.534	-53.823	158.553	1.00	34.18	S	O
	ATOM	8281	O	HOH	519	12.495	-65.958	94.103	1.00	37.35	S	O
	ATOM	8282	O	HOH	520	12.082	-63.750	158.067	1.00	40.43	S	O
55	ATOM	8283	O	HOH	521	-6.258	-14.382	107.777	1.00	34.60	S	O
	ATOM	8284	O	HOH	523	-7.698	-57.467	92.243	1.00	44.57	S	O
	ATOM	8285	O	HOH	524	-14.820	-31.957	104.702	1.00	49.92	S	O
	ATOM	8286	O	HOH	525	23.766	-78.865	111.717	1.00	49.25	S	O

-312-

5	ATOM	8287	O	HOH	526	12.535	-38.204	148.153	1.00	53.45	S	O
	ATOM	8288	O	HOH	527	-6.678	-65.953	114.241	1.00	45.88	S	O
	ATOM	8289	O	HOH	529	-21.878	-58.439	164.200	1.00	48.19	S	O
	ATOM	8290	O	HOH	530	-11.825	-37.756	116.383	1.00	45.97	S	O
	ATOM	8291	O	HOH	532	-11.859	-61.199	109.587	1.00	49.73	S	O
10	ATOM	8292	O	HOH	533	-5.953	-38.372	156.605	1.00	43.27	S	O
	ATOM	8293	O	HOH	535	-9.521	-45.912	129.467	1.00	40.80	S	O
	ATOM	8294	O	HOH	536	15.652	-33.654	161.052	1.00	39.31	S	O
	ATOM	8295	O	HOH	537	-11.557	-73.270	111.665	1.00	52.60	S	O
	ATOM	8296	O	HOH	538	14.976	-96.434	109.861	1.00	51.75	S	O
15	ATOM	8297	O	HOH	539	-6.961	-47.480	169.785	1.00	42.26	S	O
	ATOM	8298	O	HOH	540	-3.653	-40.089	169.579	1.00	44.31	S	O
	ATOM	8299	O	HOH	542	4.492	-99.754	106.625	1.00	42.46	S	O
	ATOM	8300	O	HOH	543	-15.385	-59.003	171.024	1.00	38.14	S	O
	ATOM	8301	O	HOH	544	-9.565	-39.031	162.703	1.00	43.59	S	O
20	ATOM	8302	O	HOH	545	-2.257	-14.277	104.237	1.00	51.26	S	O
	ATOM	8303	O	HOH	546	-8.109	-97.785	106.812	1.00	39.90	S	O
	ATOM	8304	O	HOH	547	7.818	-98.465	145.193	1.00	48.51	S	O
	ATOM	8305	O	HOH	548	-5.573	-51.414	122.376	1.00	47.73	S	O
	ATOM	8306	O	HOH	549	10.335	-57.290	107.995	1.00	26.18	S	O
25	ATOM	8307	O	HOH	551	-12.399	-62.220	170.747	1.00	34.90	S	O
	ATOM	8308	O	HOH	552	0.458	-16.759	105.920	1.00	50.86	S	O
	ATOM	8309	O	HOH	553	10.549	-88.842	145.088	1.00	55.30	S	O
	ATOM	8310	O	HOH	554	-19.934	-72.006	149.518	1.00	43.14	S	O
	ATOM	8311	O	HOH	555	-9.143	-35.862	147.215	1.00	44.48	S	O
30	ATOM	8312	O	HOH	557	11.968	-27.647	165.607	1.00	39.72	S	O
	ATOM	8313	O	HOH	558	7.500	-78.286	152.237	1.00	42.78	S	O
	ATOM	8314	O	HOH	559	-20.328	-67.927	149.359	1.00	42.48	S	O
	ATOM	8315	O	HOH	560	-14.589	-52.793	168.443	1.00	49.18	S	O
	ATOM	8316	O	HOH	561	14.274	-25.186	115.196	1.00	68.97	S	O
35	ATOM	8317	O	HOH	562	-11.876	-66.758	99.635	1.00	58.70	S	O
	ATOM	8318	O	HOH	563	9.652	-71.240	90.805	1.00	47.55	S	O
	ATOM	8319	O	HOH	564	8.337	-90.428	100.502	1.00	40.50	S	O
	ATOM	8320	O	HOH	565	-4.356	-37.312	154.893	1.00	45.44	S	O
	ATOM	8321	O	HOH	566	-11.188	-96.445	143.149	1.00	46.91	S	O
40	ATOM	8322	O	HOH	567	-15.389	-34.354	115.276	1.00	38.19	S	O
	ATOM	8323	O	HOH	568	-6.686	-38.757	165.227	1.00	40.62	S	O
	ATOM	8324	O	HOH	569	0.603	-92.714	105.614	1.00	49.80	S	O
	ATOM	8325	O	HOH	570	-10.908	-44.492	149.043	1.00	55.75	S	O
	ATOM	8326	O	HOH	571	11.715	-56.940	144.398	1.00	50.46	S	O
45	ATOM	8327	O	HOH	575	14.024	-39.506	110.121	1.00	77.11	S	O
	ATOM	8328	O	HOH	576	6.524	-55.615	104.387	1.00	50.00	S	O
	ATOM	8329	O	HOH	577	9.972	-97.480	121.036	1.00	48.12	S	O
	ATOM	8330	O	HOH	578	-20.801	-42.139	108.101	1.00	41.31	S	O
	ATOM	8331	O	HOH	580	-14.408	-77.621	170.420	1.00	47.84	S	O
50	ATOM	8332	O	HOH	583	18.062	-48.141	147.872	1.00	46.19	S	O
	ATOM	8333	O	HOH	584	-11.118	-38.154	93.126	1.00	52.49	S	O
	ATOM	8334	O	HOH	585	18.723	-67.355	118.436	1.00	43.61	S	O
	ATOM	8335	O	HOH	586	18.807	-22.870	147.950	1.00	49.22	S	O
	ATOM	8336	O	HOH	587	0.369	-10.834	151.620	1.00	48.37	S	O
55	ATOM	8337	O	HOH	590	-12.421	-41.425	151.484	1.00	54.81	S	O
	ATOM	8338	O	HOH	591	-6.884	-66.074	136.375	1.00	39.42	S	O
	ATOM	8339	O	HOH	592	0.492	-44.413	93.739	1.00	55.03	S	O
	ATOM	8340	O	HOH	593	6.207	-11.926	150.116	1.00	51.39	S	O
	ATOM	8341	O	HOH	594	-15.591	-54.380	154.053	1.00	44.25	S	O
	ATOM	8342	O	HOH	595	11.989	-62.147	169.236	1.00	53.46	S	O
	ATOM	8343	O	HOH	597	3.166	-80.892	136.494	1.00	41.41	S	O
	ATOM	8344	O	HOH	598	-4.024	-96.765	138.695	1.00	54.76	S	O

-313-

	ATOM	8345	O	HOH	599	4.947	-13.288	156.213	1.00	41.25	S	O
	ATOM	8346	O	HOH	601	-10.913	-56.637	111.268	1.00	50.93	S	O
	ATOM	8347	O	HOH	603	14.746	-24.982	161.752	1.00	47.50	S	O
5	ATOM	8348	O	HOH	604	5.409	-94.049	129.553	1.00	42.28	S	O
	ATOM	8349	O	HOH	605	-14.289	-47.176	126.711	1.00	52.11	S	O
	ATOM	8350	O	HOH	606	-19.924	-36.475	99.672	1.00	57.18	S	O
	ATOM	8351	O	HOH	607	17.853	-35.468	123.118	1.00	46.97	S	O
	ATOM	8352	O	HOH	608	17.766	-94.614	115.087	1.00	40.46	S	O
10	ATOM	8353	O	HOH	609	-4.020	-13.136	107.395	1.00	55.14	S	O
	ATOM	8354	O	HOH	610	-9.464	-33.125	116.432	1.00	37.22	S	O
	ATOM	8355	O	HOH	611	-10.377	-75.399	173.180	1.00	44.74	S	O
	ATOM	8356	O	HOH	612	-0.696	-90.383	133.659	1.00	45.83	S	O
	ATOM	8357	O	HOH	614	-12.440	-82.880	162.828	1.00	34.32	S	O
15	ATOM	8358	O	HOH	617	-18.663	-21.788	112.739	1.00	50.67	S	O
	ATOM	8359	O	HOH	618	-18.590	-57.120	169.501	1.00	48.06	S	O
	ATOM	8360	O	HOH	619	-20.062	-92.620	148.628	1.00	54.49	S	O
	ATOM	8361	O	HOH	620	-15.408	-66.228	136.844	1.00	53.29	S	O
	ATOM	8362	O	HOH	621	10.798	-68.875	164.880	1.00	46.75	S	O
20	ATOM	8363	O	HOH	623	9.041	-99.725	148.740	1.00	58.12	S	O
	ATOM	8364	O	HOH	626	9.984	-17.186	146.410	1.00	52.87	S	O
	ATOM	8365	O	HOH	627	-5.441	-12.548	128.206	1.00	61.98	S	O
	ATOM	8366	O	HOH	628	14.243	-48.135	170.673	1.00	41.69	S	O
	ATOM	8367	O	HOH	629	0.255	-80.174	155.302	1.00	39.69	S	O
25	ATOM	8368	O	HOH	630	-7.005	-18.269	116.783	1.00	48.41	S	O
	ATOM	8369	O	HOH	631	10.537	-29.846	165.191	1.00	46.58	S	O
	ATOM	8370	O	HOH	633	16.493	-46.188	169.718	1.00	41.32	S	O
	ATOM	8371	O	HOH	634	1.296	-11.323	111.912	1.00	48.12	S	O
	ATOM	8372	O	HOH	635	-10.380	-57.565	95.694	1.00	32.16	S	O
30	ATOM	8373	O	HOH	636	-20.531	-82.493	147.829	1.00	42.76	S	O
	ATOM	8374	O	HOH	637	-5.588	-69.902	122.015	1.00	37.58	S	O
	ATOM	8375	O	HOH	638	5.861	-81.002	152.992	1.00	55.36	S	O
	ATOM	8376	O	HOH	639	-1.444	-80.158	108.941	1.00	40.46	S	O
	ATOM	8377	O	HOH	640	-12.826	-31.755	98.733	1.00	55.93	S	O
35	ATOM	8378	O	HOH	641	-12.041	-90.235	104.096	1.00	48.46	S	O
	ATOM	8379	O	HOH	642	-22.335	-75.465	150.732	1.00	50.86	S	O
	ATOM	8380	O	HOH	643	14.088	-18.781	123.781	1.00	49.25	S	O
	ATOM	8381	O	HOH	644	-8.248	-95.373	103.761	1.00	53.33	S	O
	ATOM	8382	O	HOH	645	-8.607	-32.918	166.992	1.00	59.33	S	O
40	ATOM	8383	O	HOH	646	5.063	-70.803	169.143	1.00	50.88	S	O
	ATOM	8384	O	HOH	647	16.334	-45.651	141.775	1.00	62.45	S	O
	ATOM	8385	O	HOH	648	-5.014	-44.649	141.840	1.00	53.76	S	O
	ATOM	8386	O	HOH	649	-13.704	-26.229	101.833	1.00	51.97	S	O
	ATOM	8387	O	HOH	651	8.563	-18.798	147.662	1.00	44.65	S	O
45	ATOM	8388	O	HOH	653	-9.912	-68.068	134.022	1.00	53.05	S	O
	ATOM	8389	O	HOH	655	-0.311	-71.123	138.891	1.00	54.56	S	O
	ATOM	8390	O	HOH	656	-16.546	-46.675	121.208	1.00	50.84	S	O
	ATOM	8391	O	HOH	658	-2.023	-57.281	144.738	1.00	47.88	S	O
	ATOM	8392	O	HOH	659	14.501	-77.574	110.573	1.00	41.41	S	O
50	ATOM	8393	O	HOH	661	16.983	-82.991	102.774	1.00	47.84	S	O
	ATOM	8394	O	HOH	663	10.061	-75.062	90.477	1.00	52.90	S	O
	ATOM	8395	O	HOH	664	15.100	-47.917	101.333	1.00	57.41	S	O
	ATOM	8396	O	HOH	668	-3.335	-45.148	170.230	1.00	51.20	S	O
	ATOM	8397	O	HOH	672	-15.814	-49.740	160.931	1.00	52.16	S	O
55	ATOM	8398	O	HOH	673	-12.012	-62.301	106.971	1.00	62.83	S	O
	ATOM	8399	O	HOH	674	13.451	-56.883	106.975	1.00	43.13	S	O
	ATOM	8400	O	HOH	676	8.821	-29.261	110.887	1.00	43.22	S	O
	ATOM	8401	O	HOH	677	-2.141	-11.541	104.475	1.00	45.96	S	O
	ATOM	8402	O	HOH	681	-10.652	-35.075	160.241	1.00	52.13	S	O

-314-

	ATOM	8403	O	HOH	685	-0.033	-82.942	139.985	1.00	54.94	S	O
	ATOM	8404	O	HOH	686	-12.713	-15.439	118.692	1.00	70.33	S	O
	ATOM	8405	O	HOH	689	-10.374	-96.022	146.296	1.00	55.51	S	O
5	ATOM	8406	O	HOH	690	-15.464	-57.285	111.706	1.00	50.64	S	O
	ATOM	8407	O	HOH	691	11.081	-60.842	125.875	1.00	68.98	S	O
	ATOM	8408	O	HOH	692	6.707	-44.563	122.251	1.00	52.71	S	O
	ATOM	8409	O	HOH	693	-9.745	-94.906	137.556	1.00	42.37	S	O
	ATOM	8410	O	HOH	695	-1.304	-62.997	120.562	1.00	43.89	S	O
10	ATOM	8411	O	HOH	697	0.730	-62.955	144.181	1.00	67.72	S	O
	ATOM	8412	O	HOH	698	-3.780	-84.834	96.026	1.00	68.94	S	O
	ATOM	8413	O	HOH	701	-19.964	-55.244	155.074	1.00	70.97	S	O
	ATOM	8414	O	HOH	702	-17.043	-70.577	133.458	1.00	52.11	S	O
	ATOM	8415	O	HOH	703	-4.439	-29.599	138.511	1.00	44.42	S	O
15	ATOM	8416	O	HOH	708	-13.381	-34.208	97.616	1.00	54.25	S	O
	ATOM	8417	O	HOH	709	-17.495	-54.498	158.139	1.00	55.23	S	O
	ATOM	8418	O	HOH	714	2.274	-18.552	158.773	1.00	43.63	S	O
	ATOM	8419	O	HOH	719	-2.397	-85.569	126.958	1.00	51.95	S	O
	ATOM	8420	O	HOH	723	16.887	-97.297	117.416	1.00	57.09	S	O
20	ATOM	8421	O	HOH	725	-20.095	-93.695	156.379	1.00	48.48	S	O
	ATOM	8422	O	HOH	728	-20.097	-34.574	98.029	1.00	45.93	S	O
	ATOM	8423	O	HOH	730	5.820	-62.677	172.241	1.00	52.85	S	O
	ATOM	8424	O	HOH	733	14.590	-77.427	94.470	1.00	48.88	S	O
	ATOM	8425	O	HOH	734	-9.869	-22.276	134.367	1.00	72.16	S	O
25	ATOM	8426	O	HOH	735	5.303	-36.085	129.231	1.00	30.02	S	O
	ATOM	8427	O	HOH	736	3.098	-34.827	125.987	1.00	26.22	S	O
	ATOM	8428	O	HOH	737	10.874	-90.931	100.638	1.00	41.15	S	O
	ATOM	8429	O	HOH	738	-23.151	-61.565	160.742	1.00	32.42	S	O
	ATOM	8430	O	HOH	739	-8.831	-59.000	93.865	1.00	32.91	S	O
30	ATOM	8431	O	HOH	741	6.367	-55.107	150.140	1.00	25.10	S	O
	ATOM	8432	O	HOH	742	1.837	-77.812	155.807	1.00	40.46	S	O
	ATOM	8433	O	HOH	743	18.373	-59.937	105.014	1.00	40.07	S	O
	ATOM	8434	O	HOH	744	-8.704	-56.710	105.086	1.00	29.75	S	O
	ATOM	8435	O	HOH	745	-7.231	-63.368	144.159	1.00	34.27	S	O
35	ATOM	8436	O	HOH	746	12.259	-58.932	105.752	1.00	34.90	S	O
	ATOM	8437	O	HOH	747	-7.099	-93.546	162.206	1.00	31.38	S	O
	ATOM	8438	O	HOH	748	14.860	-52.071	107.364	1.00	43.45	S	O
	ATOM	8439	O	HOH	749	-16.011	-39.637	98.635	1.00	60.23	S	O
	ATOM	8440	O	HOH	750	-1.736	-100.443	157.176	1.00	35.25	S	O
40	ATOM	8441	O	HOH	751	-17.531	-32.113	130.416	1.00	51.18	S	O
	ATOM	8442	O	HOH	756	12.661	-14.091	135.708	1.00	70.13	S	O
	ATOM	8443	O	HOH	760	15.150	-22.603	154.565	1.00	51.07	S	O
	ATOM	8444	O	HOH	768	9.497	-28.553	123.786	1.00	58.62	S	O
	ATOM	8445	O	HOH	770	-4.253	-31.597	135.470	1.00	48.19	S	O
45	ATOM	8446	O	HOH	771	11.018	-64.258	168.175	1.00	49.12	S	O
	ATOM	8447	O	HOH	773	-1.147	-18.922	105.507	1.00	49.76	S	O
	ATOM	8448	O	HOH	774	-1.791	-79.776	101.201	1.00	56.64	S	O
	ATOM	8449	O	HOH	775	17.234	-83.652	115.724	1.00	55.57	S	O
	ATOM	8450	O	HOH	776	-9.749	-49.262	92.864	1.00	33.00	S	O
50	ATOM	8451	O	HOH	777	-23.197	-63.886	160.148	1.00	54.59	S	O
	ATOM	8452	O	HOH	778	-6.093	-55.694	160.150	1.00	47.65	S	O
	ATOM	8453	O	HOH	779	17.290	-20.496	151.229	1.00	42.84	S	O
	ATOM	8454	O	HOH	783	-18.249	-55.806	106.538	1.00	55.53	S	O
	ATOM	8455	O	HOH	784	-2.720	-79.830	125.976	1.00	22.05	S	O
55	ATOM	8456	O	HOH	785	8.349	-35.548	129.815	1.00	28.26	S	O
	ATOM	8457	O	HOH	786	-8.539	-78.807	129.222	1.00	29.66	S	O
	ATOM	8458	O	HOH	787	-4.322	-35.630	134.871	1.00	40.03	S	O
	ATOM	8459	O	HOH	788	-17.713	-86.008	159.140	1.00	34.22	S	O
	ATOM	8460	O	HOH	789	11.187	-59.273	158.430	1.00	33.45	S	O

-315-

	ATOM	8461	O	HOH	790	-15.720	-76.210	153.508	1.00	36.09	S	O
	ATOM	8462	O	HOH	791	16.504	-32.487	159.130	1.00	44.35	S	O
	ATOM	8463	O	HOH	795	-15.122	-86.248	165.186	1.00	37.18	S	O
5	ATOM	8464	O	HOH	802	1.557	-43.210	127.554	1.00	61.28	S	O
	ATOM	8465	O	HOH	804	-8.966	-52.044	92.549	1.00	27.57	S	O
	ATOM	8466	O	HOH	805	16.463	-36.887	145.786	1.00	39.77	S	O
	ATOM	8467	O	HOH	806	1.720	-46.690	140.997	1.00	45.60	S	O
	ATOM	8468	O	HOH	807	-14.220	-55.032	166.003	1.00	27.66	S	O
10	ATOM	8469	O	HOH	808	-10.216	-54.376	157.359	1.00	36.07	S	O
	TER	8470		HOH	808						S	
	ATOM	8471	C1	596	1	-2.438	-45.928	106.741	1.00	18.61	L	C
	ATOM	8472	N2	596	1	-2.499	-44.805	105.931	1.00	19.75	L	N
	ATOM	8473	C3	596	1	-1.360	-45.713	107.663	1.00	19.36	L	C
15	ATOM	8474	C4	596	1	-3.196	-47.099	106.859	1.00	19.46	L	C
	ATOM	8475	C5	596	1	-1.505	-44.003	106.355	1.00	20.57	L	C
	ATOM	8476	C6	596	1	-3.571	-44.495	104.958	1.00	18.69	L	C
	ATOM	8477	N7	596	1	-0.807	-44.501	107.372	1.00	19.90	L	N
	ATOM	8478	C8	596	1	-1.092	-46.669	108.636	1.00	18.27	L	C
20	ATOM	8479	C9	596	1	-2.938	-48.091	107.869	1.00	19.94	L	C
	ATOM	8480	N10	596	1	-1.251	-42.680	105.817	1.00	22.09	L	N
	ATOM	8481	C11	596	1	-4.572	-43.441	105.486	1.00	18.66	L	C
	ATOM	8482	C12	596	1	-1.865	-47.853	108.767	1.00	19.06	L	C
	ATOM	8483	C13	596	1	-3.702	-49.316	108.040	1.00	20.54	L	C
25	ATOM	8484	C14	596	1	-0.260	-41.769	106.410	1.00	23.52	L	C
	ATOM	8485	C15	596	1	-5.361	-43.944	106.666	1.00	18.98	L	C
	ATOM	8486	N16	596	1	-4.949	-49.325	107.482	1.00	20.47	L	N
	ATOM	8487	O17	596	1	-3.260	-50.270	108.680	1.00	21.54	L	O
	ATOM	8488	C18	596	1	-0.883	-40.381	106.319	1.00	23.09	L	C
30	ATOM	8489	C19	596	1	1.195	-41.956	105.908	1.00	23.60	L	C
	ATOM	8490	C20	596	1	-4.909	-43.722	107.977	1.00	19.73	L	C
	ATOM	8491	C21	596	1	-6.489	-44.737	106.476	1.00	18.94	L	C
	ATOM	8492	C22	596	1	-1.972	-40.125	107.159	1.00	23.10	L	C
	ATOM	8493	C23	596	1	-0.463	-39.357	105.437	1.00	23.56	L	C
35	ATOM	8494	C24	596	1	1.522	-42.897	104.908	1.00	23.72	L	C
	ATOM	8495	C25	596	1	2.255	-41.178	106.433	1.00	23.90	L	C
	ATOM	8496	C26	596	1	-5.540	-44.354	109.074	1.00	20.03	L	C
	ATOM	8497	C27	596	1	-7.135	-45.348	107.563	1.00	19.94	L	C
	ATOM	8498	C28	596	1	-2.669	-38.914	107.082	1.00	23.17	L	C
40	ATOM	8499	C29	596	1	-1.144	-38.130	105.363	1.00	23.29	L	C
	ATOM	8500	C30	596	1	2.822	-43.019	104.418	1.00	24.28	L	C
	ATOM	8501	C31	596	1	3.560	-41.277	105.906	1.00	24.30	L	C
	ATOM	8502	C32	596	1	-6.666	-45.165	108.860	1.00	19.58	L	C
	ATOM	8503	C33	596	1	-2.254	-37.917	106.184	1.00	23.09	L	C
45	ATOM	8504	C34	596	1	3.826	-42.181	104.890	1.00	23.94	L	C
	ATOM	8505	H35	596	1	-4.001	-47.227	106.157	1.00	19.63	L	H
	ATOM	8506	H36	596	1	-4.110	-45.386	104.677	1.00	19.04	L	H
	ATOM	8507	H37	596	1	-3.110	-44.126	104.055	1.00	19.09	L	H
	ATOM	8508	H38	596	1	-0.255	-46.507	109.290	1.00	18.86	L	H
50	ATOM	8509	H39	596	1	-1.822	-42.349	105.069	1.00	22.39	L	H
	ATOM	8510	H40	596	1	-5.258	-43.176	104.699	1.00	18.82	L	H
	ATOM	8511	H41	596	1	-4.060	-42.538	105.768	1.00	18.85	L	H
	ATOM	8512	H42	596	1	-1.654	-48.568	109.542	1.00	19.54	L	H
	ATOM	8513	H43	596	1	-0.233	-41.991	107.467	1.00	23.34	L	H
55	ATOM	8514	H44	596	1	-5.303	-48.517	107.008	1.00	20.75	L	H
	ATOM	8515	H45	596	1	-5.503	-50.155	107.553	1.00	20.71	L	H
	ATOM	8516	H46	596	1	-4.031	-43.115	108.126	1.00	19.63	L	H
	ATOM	8517	H47	596	1	-6.864	-44.900	105.478	1.00	19.30	L	H
	ATOM	8518	H48	596	1	-2.277	-40.857	107.889	1.00	23.21	L	H

-316-

5	ATOM	8519	H49	596	1	0.389	-39.503	104.794	1.00	23.37	L	H
	ATOM	8520	H50	596	1	0.781	-43.548	104.470	1.00	23.80	L	H
	ATOM	8521	H51	596	1	2.062	-40.480	107.234	1.00	23.82	L	H
	ATOM	8522	H52	596	1	-5.160	-44.208	110.074	1.00	19.98	L	H
10	ATOM	8523	H53	596	1	-8.005	-45.966	107.398	1.00	19.79	L	H
	ATOM	8524	H54	596	1	-3.517	-38.756	107.729	1.00	23.18	L	H
	ATOM	8525	H55	596	1	-0.814	-37.365	104.678	1.00	23.37	L	H
	ATOM	8526	H56	596	1	3.034	-43.752	103.657	1.00	24.22	L	H
15	ATOM	8527	H57	596	1	4.359	-40.656	106.289	1.00	24.15	L	H
	ATOM	8528	H58	596	1	-7.176	-45.633	109.685	1.00	19.69	L	H
	ATOM	8529	H59	596	1	-2.788	-36.980	106.143	1.00	23.46	L	H
	ATOM	8530	H60	596	1	4.809	-42.244	104.457	1.00	24.48	L	H
20	ATOM	8531	C1	596	2	4.336	-69.170	106.987	1.00	17.81	R	C
	ATOM	8532	N2	596	2	4.440	-70.327	106.207	1.00	17.06	R	N
	ATOM	8533	C3	596	2	3.162	-69.331	107.787	1.00	18.16	R	C
	ATOM	8534	C4	596	2	5.127	-68.030	107.183	1.00	17.87	R	C
25	ATOM	8535	C5	596	2	3.405	-71.098	106.552	1.00	17.68	R	C
	ATOM	8536	C6	596	2	5.586	-70.634	105.341	1.00	16.75	R	C
	ATOM	8537	N7	596	2	2.635	-70.555	107.475	1.00	18.02	R	N
	ATOM	8538	C8	596	2	2.820	-68.344	108.702	1.00	17.84	R	C
30	ATOM	8539	C9	596	2	4.789	-67.013	108.148	1.00	18.61	R	C
	ATOM	8540	N10	596	2	3.123	-72.420	106.004	1.00	18.38	R	N
	ATOM	8541	C11	596	2	6.546	-71.662	105.985	1.00	16.15	R	C
	ATOM	8542	C12	596	2	3.605	-67.184	108.904	1.00	17.98	R	C
35	ATOM	8543	C13	596	2	5.614	-65.865	108.504	1.00	18.62	R	C
	ATOM	8544	C14	596	2	2.047	-73.304	106.474	1.00	18.34	R	C
	ATOM	8545	C15	596	2	7.255	-71.129	107.206	1.00	16.15	R	C
	ATOM	8546	N16	596	2	6.925	-65.908	108.153	1.00	18.90	R	N
40	ATOM	8547	O17	596	2	5.159	-64.930	109.159	1.00	20.09	R	O
	ATOM	8548	C18	596	2	2.661	-74.677	106.388	1.00	17.44	R	C
	ATOM	8549	C19	596	2	0.683	-73.086	105.780	1.00	20.03	R	C
	ATOM	8550	C20	596	2	6.750	-71.375	108.506	1.00	16.48	R	C
45	ATOM	8551	C21	596	2	8.371	-70.304	107.048	1.00	15.06	R	C
	ATOM	8552	C22	596	2	3.682	-74.969	107.305	1.00	16.86	R	C
	ATOM	8553	C23	596	2	2.335	-75.659	105.424	1.00	17.31	R	C
	ATOM	8554	C24	596	2	0.509	-72.121	104.758	1.00	19.86	R	C
50	ATOM	8555	C25	596	2	-0.458	-73.856	106.157	1.00	21.14	R	C
	ATOM	8556	C26	596	2	7.309	-70.703	109.617	1.00	16.65	R	C
	ATOM	8557	C27	596	2	8.953	-69.660	108.142	1.00	15.10	R	C
	ATOM	8558	C28	596	2	4.378	-76.188	107.242	1.00	16.83	R	C
55	ATOM	8559	C29	596	2	3.005	-76.891	105.375	1.00	17.45	R	C
	ATOM	8560	C30	596	2	-0.709	-71.956	104.108	1.00	21.12	R	C
	ATOM	8561	C31	596	2	-1.677	-73.701	105.487	1.00	22.11	R	C
	ATOM	8562	C32	596	2	8.415	-69.847	109.421	1.00	16.40	R	C
55	ATOM	8563	C33	596	2	4.039	-77.149	106.291	1.00	17.12	R	C
	ATOM	8564	C34	596	2	-1.801	-72.758	104.454	1.00	21.79	R	C
	ATOM	8565	H35	596	2	6.024	-67.954	106.594	1.00	18.11	R	H
	ATOM	8566	H36	596	2	6.161	-69.749	105.110	1.00	16.89	R	H
55	ATOM	8567	H37	596	2	5.191	-71.000	104.403	1.00	16.85	R	H
	ATOM	8568	H38	596	2	1.936	-68.493	109.299	1.00	18.19	R	H
	ATOM	8569	H39	596	2	3.705	-72.773	105.274	1.00	18.51	R	H
	ATOM	8570	H40	596	2	7.293	-71.922	105.252	1.00	16.39	R	H
55	ATOM	8571	H41	596	2	6.008	-72.564	106.242	1.00	16.29	R	H
	ATOM	8572	H42	596	2	3.345	-66.465	109.657	1.00	18.45	R	H
	ATOM	8573	H43	596	2	1.907	-73.105	107.522	1.00	18.65	R	H
	ATOM	8574	H44	596	2	7.302	-66.689	107.652	1.00	19.02	R	H
55	ATOM	8575	H45	596	2	7.510	-65.137	108.408	1.00	19.09	R	H
	ATOM	8576	H46	596	2	5.903	-72.034	108.633	1.00	16.43	R	H

-317-

5	ATOM	8577	H47	596	2	8.758	-70.133	106.057	1.00	15.62	R	H
	ATOM	8578	H48	596	2	3.925	-74.260	108.081	1.00	16.88	R	H
	ATOM	8579	H49	596	2	1.556	-75.498	104.697	1.00	17.51	R	H
	ATOM	8580	H50	596	2	1.310	-71.479	104.438	1.00	20.27	R	H
	ATOM	8581	H51	596	2	-0.390	-74.586	106.951	1.00	21.25	R	H
10	ATOM	8582	H52	596	2	6.891	-70.827	110.605	1.00	16.51	R	H
	ATOM	8583	H53	596	2	9.797	-69.006	108.010	1.00	15.29	R	H
	ATOM	8584	H54	596	2	5.161	-76.405	107.946	1.00	17.12	R	H
	ATOM	8585	H55	596	2	2.723	-77.634	104.647	1.00	17.47	R	H
	ATOM	8586	H56	596	2	-0.806	-71.205	103.339	1.00	21.25	R	H
15	ATOM	8587	H57	596	2	-2.512	-74.336	105.751	1.00	22.07	R	H
	ATOM	8588	H58	596	2	8.852	-69.329	110.259	1.00	16.27	R	H
	ATOM	8589	H59	596	2	4.558	-78.095	106.287	1.00	17.47	R	H
	ATOM	8590	H60	596	2	-2.735	-72.657	103.923	1.00	21.89	R	H
	ATOM	8591	C1	596	3	2.846	-46.116	157.632	1.00	15.32	T	C
20	ATOM	8592	N2	596	3	2.939	-44.983	158.430	1.00	16.26	T	N
	ATOM	8593	C3	596	3	1.752	-45.890	156.704	1.00	15.57	T	C
	ATOM	8594	C4	596	3	3.601	-47.287	157.515	1.00	14.61	T	C
	ATOM	8595	C5	596	3	1.945	-44.165	157.987	1.00	16.95	T	C
	ATOM	8596	C6	596	3	4.027	-44.670	159.405	1.00	15.77	T	C
25	ATOM	8597	N7	596	3	1.214	-44.671	156.986	1.00	14.76	T	N
	ATOM	8598	C8	596	3	1.501	-46.839	155.702	1.00	14.30	T	C
	ATOM	8599	C9	596	3	3.340	-48.270	156.482	1.00	15.09	T	C
	ATOM	8600	N10	596	3	1.720	-42.818	158.524	1.00	16.85	T	N
	ATOM	8601	C11	596	3	5.028	-43.656	158.829	1.00	15.65	T	C
30	ATOM	8602	C12	596	3	2.274	-48.030	155.565	1.00	14.20	T	C
	ATOM	8603	C13	596	3	4.091	-49.540	156.364	1.00	13.71	T	C
	ATOM	8604	C14	596	3	0.792	-41.854	157.922	1.00	16.81	T	C
	ATOM	8605	C15	596	3	5.841	-44.235	157.706	1.00	16.86	T	C
	ATOM	8606	N16	596	3	5.327	-49.545	156.931	1.00	12.82	T	N
35	ATOM	8607	O17	596	3	3.620	-50.530	155.803	1.00	12.64	T	O
	ATOM	8608	C18	596	3	1.529	-40.533	157.929	1.00	15.58	T	C
	ATOM	8609	C19	596	3	-0.633	-41.901	158.482	1.00	16.81	T	C
	ATOM	8610	C20	596	3	5.446	-44.048	156.366	1.00	17.32	T	C
	ATOM	8611	C21	596	3	6.943	-45.071	157.971	1.00	17.36	T	C
40	ATOM	8612	C22	596	3	2.526	-40.356	156.970	1.00	15.60	T	C
	ATOM	8613	C23	596	3	1.327	-39.508	158.869	1.00	15.97	T	C
	ATOM	8614	C24	596	3	-1.027	-42.802	159.499	1.00	17.21	T	C
	ATOM	8615	C25	596	3	-1.623	-41.014	157.976	1.00	17.34	T	C
	ATOM	8616	C26	596	3	6.087	-44.738	155.318	1.00	17.94	T	C
45	ATOM	8617	C27	596	3	7.605	-45.724	156.911	1.00	18.26	T	C
	ATOM	8618	C28	596	3	3.327	-39.207	156.961	1.00	15.61	T	C
	ATOM	8619	C29	596	3	2.072	-38.320	158.836	1.00	16.06	T	C
	ATOM	8620	C30	596	3	-2.333	-42.774	160.051	1.00	17.06	T	C
	ATOM	8621	C31	596	3	-2.922	-40.988	158.511	1.00	17.58	T	C
50	ATOM	8622	C32	596	3	7.181	-45.565	155.595	1.00	17.92	T	C
	ATOM	8623	C33	596	3	3.089	-38.180	157.872	1.00	15.78	T	C
	ATOM	8624	C34	596	3	-3.260	-41.857	159.552	1.00	17.41	T	C
	ATOM	8625	H35	596	3	4.396	-47.438	158.229	1.00	14.89	T	H
	ATOM	8626	H36	596	3	4.548	-45.560	159.719	1.00	16.02	T	H
55	ATOM	8627	H37	596	3	3.570	-44.278	160.303	1.00	16.08	T	H
	ATOM	8628	H38	596	3	0.716	-46.615	154.998	1.00	14.65	T	H
	ATOM	8629	H39	596	3	2.263	-42.518	159.303	1.00	17.20	T	H
	ATOM	8630	H40	596	3	5.704	-43.349	159.607	1.00	16.13	T	H
	ATOM	8631	H41	596	3	4.522	-42.767	158.496	1.00	16.08	T	H
	ATOM	8632	H42	596	3	2.065	-48.754	154.791	1.00	14.79	T	H
	ATOM	8633	H43	596	3	0.714	-42.122	156.879	1.00	16.80	T	H
	ATOM	8634	H44	596	3	5.710	-48.742	157.389	1.00	12.65	T	H

-318-

5	ATOM	8635	H45	596	3	5.897	-50.359	156.902	1.00	12.70	T	H
	ATOM	8636	H46	596	3	4.608	-43.403	156.149	1.00	17.56	T	H
	ATOM	8637	H47	596	3	7.264	-45.259	158.984	1.00	17.47	T	H
	ATOM	8638	H48	596	3	2.702	-41.118	156.226	1.00	15.78	T	H
	ATOM	8639	H49	596	3	0.601	-39.633	159.657	1.00	16.06	T	H
10	ATOM	8640	H50	596	3	-0.332	-43.510	159.920	1.00	17.16	T	H
	ATOM	8641	H51	596	3	-1.367	-40.340	157.175	1.00	17.30	T	H
	ATOM	8642	H52	596	3	5.751	-44.629	154.301	1.00	17.79	T	H
	ATOM	8643	H53	596	3	8.440	-46.371	157.117	1.00	18.15	T	H
	ATOM	8644	H54	596	3	4.123	-39.108	156.244	1.00	15.83	T	H
15	ATOM	8645	H55	596	3	1.875	-37.532	159.550	1.00	15.79	T	H
	ATOM	8646	H56	596	3	-2.598	-43.416	160.883	1.00	17.05	T	H
	ATOM	8647	H57	596	3	-3.658	-40.295	158.132	1.00	17.59	T	H
	ATOM	8648	H58	596	3	7.699	-46.063	154.797	1.00	18.12	T	H
	ATOM	8649	H59	596	3	3.682	-37.276	157.832	1.00	15.95	T	H
20	ATOM	8650	H60	596	3	-4.247	-41.800	159.990	1.00	17.61	T	H
	ATOM	8651	C1	596	4	-5.000	-68.974	157.356	1.00	15.41	V	C
	ATOM	8652	N2	596	4	-5.233	-70.123	158.103	1.00	15.55	V	N
	ATOM	8653	C3	596	4	-3.819	-69.217	156.559	1.00	16.29	V	C
	ATOM	8654	C4	596	4	-5.680	-67.768	157.185	1.00	15.23	V	C
25	ATOM	8655	C5	596	4	-4.254	-70.970	157.751	1.00	17.80	V	C
	ATOM	8656	C6	596	4	-6.387	-70.373	158.973	1.00	14.78	V	C
	ATOM	8657	N7	596	4	-3.400	-70.481	156.854	1.00	17.03	V	N
	ATOM	8658	C8	596	4	-3.357	-68.243	155.667	1.00	15.66	V	C
	ATOM	8659	C9	596	4	-5.230	-66.775	156.248	1.00	16.16	V	C
30	ATOM	8660	N10	596	4	-4.114	-72.308	158.283	1.00	19.21	V	N
	ATOM	8661	C11	596	4	-7.439	-71.298	158.336	1.00	15.05	V	C
	ATOM	8662	C12	596	4	-4.037	-67.015	155.502	1.00	15.69	V	C
	ATOM	8663	C13	596	4	-5.921	-65.520	155.976	1.00	15.40	V	C
	ATOM	8664	C14	596	4	-3.153	-73.285	157.784	1.00	20.54	V	C
35	ATOM	8665	C15	596	4	-8.089	-70.681	157.105	1.00	14.31	V	C
	ATOM	8666	N16	596	4	-7.227	-65.478	156.246	1.00	15.48	V	N
	ATOM	8667	O17	596	4	-5.343	-64.575	155.454	1.00	16.46	V	O
	ATOM	8668	C18	596	4	-3.861	-74.624	157.842	1.00	20.15	V	C
	ATOM	8669	C19	596	4	-1.778	-73.205	158.435	1.00	21.79	V	C
40	ATOM	8670	C20	596	4	-7.554	-70.955	155.847	1.00	14.50	V	C
	ATOM	8671	C21	596	4	-9.172	-69.808	157.201	1.00	13.56	V	C
	ATOM	8672	C22	596	4	-4.843	-74.838	156.878	1.00	19.47	V	C
	ATOM	8673	C23	596	4	-3.638	-75.621	158.809	1.00	20.11	V	C
	ATOM	8674	C24	596	4	-1.491	-72.278	159.483	1.00	22.05	V	C
45	ATOM	8675	C25	596	4	-0.733	-74.027	157.954	1.00	22.52	V	C
	ATOM	8676	C26	596	4	-8.034	-70.297	154.701	1.00	15.23	V	C
	ATOM	8677	C27	596	4	-9.702	-69.180	156.046	1.00	14.11	V	C
	ATOM	8678	C28	596	4	-5.604	-76.022	156.897	1.00	20.11	V	C
	ATOM	8679	C29	596	4	-4.370	-76.816	158.792	1.00	19.91	V	C
50	ATOM	8680	C30	596	4	-0.221	-72.173	160.033	1.00	22.72	V	C
	ATOM	8681	C31	596	4	0.545	-73.914	158.513	1.00	23.89	V	C
	ATOM	8682	C32	596	4	-9.128	-69.413	154.798	1.00	14.57	V	C
	ATOM	8683	C33	596	4	-5.362	-77.014	157.857	1.00	19.08	V	C
	ATOM	8684	C34	596	4	0.796	-72.998	159.561	1.00	23.31	V	C
55	ATOM	8685	H35	596	4	-6.566	-67.610	157.776	1.00	15.39	V	H
	ATOM	8686	H36	596	4	-6.869	-69.448	159.250	1.00	15.16	V	H
	ATOM	8687	H37	596	4	-6.028	-70.812	159.890	1.00	15.23	V	H
	ATOM	8688	H38	596	4	-2.462	-68.432	155.105	1.00	15.91	V	H
	ATOM	8689	H39	596	4	-4.759	-72.600	158.987	1.00	19.56	V	H
	ATOM	8690	H40	596	4	-8.212	-71.526	159.057	1.00	14.81	V	H
	ATOM	8691	H41	596	4	-6.976	-72.235	158.063	1.00	14.91	V	H
	ATOM	8692	H42	596	4	-3.664	-66.262	154.828	1.00	16.36	V	H

-319-

5	ATOM	8693	H43	596	4	-3.023	-73.063	156.736	1.00	20.49	V	H
	ATOM	8694	H44	596	4	-7.674	-66.265	156.678	1.00	15.81	V	H
	ATOM	8695	H45	596	4	-7.746	-64.660	156.003	1.00	15.79	V	H
	ATOM	8696	H46	596	4	-6.745	-71.667	155.781	1.00	14.88	V	H
	ATOM	8697	H47	596	4	-9.601	-69.601	158.167	1.00	14.04	V	H
10	ATOM	8698	H48	596	4	-5.019	-74.086	156.124	1.00	19.70	V	H
	ATOM	8699	H49	596	4	-2.932	-75.479	159.612	1.00	20.34	V	H
	ATOM	8700	H50	596	4	-2.242	-71.633	159.911	1.00	22.23	V	H
	ATOM	8701	H51	596	4	-0.914	-74.727	157.153	1.00	22.61	V	H
	ATOM	8702	H52	596	4	-7.560	-70.482	153.747	1.00	15.36	V	H
15	ATOM	8703	H53	596	4	-10.538	-68.503	156.125	1.00	14.26	V	H
	ATOM	8704	H54	596	4	-6.380	-76.155	156.163	1.00	19.84	V	H
	ATOM	8705	H55	596	4	-4.177	-77.575	159.533	1.00	20.19	V	H
	ATOM	8706	H56	596	4	-0.042	-71.464	160.825	1.00	23.01	V	H
	ATOM	8707	H57	596	4	1.346	-74.536	158.135	1.00	23.57	V	H
	ATOM	8708	H58	596	4	-9.501	-68.923	153.917	1.00	14.82	V	H
	ATOM	8709	H59	596	4	-5.939	-77.923	157.887	1.00	19.84	V	H
	ATOM	8710	H60	596	4	1.775	-72.930	160.006	1.00	23.48	V	H

-320-

References

The references listed below as well as all references cited in the specification are incorporated herein by reference to the extent that they supplement, explain, provide a background for or teach methodology, techniques and/or compositions employed herein.

Adams PD, Pannu NS, Read RJ & Brunger AT (1997) Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement. *Proc Natl Acad Sci U S A* 94: 5018-23.

Altschul SF, Gish W, Miller W, Myers EW & Lipman DJ (1990) Basic Local Alignment Search Tool, *J Mol Biol* 215:403-410.

Agrawal S, ed., (1993) Protocols for Oligonucleotides and Analogs: Synthesis and Properties: Methods in Molecular Biology, volume 20, Humana Press, Totowa, New Jersey, United States of America.

Allen FH, Kennard O, Motherwell DS, Town WG, Watson DG (1973) The Cambridge Crystallographic Structural Data File. *J. Chem. Doc.* 13: 119.

Amemiya Y (1997) Methods in Enzymology, Vol. 276, pp. 233-243 Academic Press, San Diego, California, United States of America.

Appelt K (1993) *Perspectives in Drug Discovery and Design* 1:23-48.

Ausubel FM, Brent R, Kingston RE, Moore DD, Seidman JG, Smith JA & Struhl K, eds (1994) Current Protocols in Molecular Biology. Wiley, New York, United States of America.

Baes M, Gulick T, Choi HS, Martinoli MG, Simha D & Moore DD (1994) A New Orphan Member of the Nuclear Hormone Receptor Superfamily That Interacts with a Subset of Retinoic Acid Response Elements, *Mol Cell Biol* 14:1544-1551.

Bartlett *et al.* (1989) *Special Pub., Royal Chem. Soc.* 78: 182-196.

Beato M, Herrlich P & Schutz G (1995) Steroid Hormone Receptors: Many Actors in Search of a Plot, *Cell* 83:851-857.

Blundell & Johnson (1985) *Meth Enzymol*, 114A & 115B, Wyckoff *et al.*, eds., Academic Press, San Diego, California, United States of America.

-321-

Blundell T, Carney D, Gardner S, Hayes F, Howlin B, Hubbard T, Overington J, Singh DA, Sibanda BL & Sutcliffe M (1988) 18th Sir Hans Krebs lecture. Knowledge-based protein modelling and design. *Eur J Biochem* 172:513-520.

5 Bohm, J *Comput Aid Mol Des*, 6: 61-78, 1992.

Bondi A, *J Phys Chem*, 68: 441-451, 1964.

Boobbyer DN, Goodford PJ, McWhinnie PM & Wade RC (1989) New hydrogen-bond potentials for use in determining energetically favorable binding sites on molecules of known structure. *J Med Chem* 32:1083-1094.

10 Bowie JU, Luthy R & Eisenberg D (1991) A method to identify protein sequences that fold into a known three-dimensional structure. *Science* 253: 164-170.

Brint AT & Willett P (1987) Pharmacophoric pattern matching in files of 3D chemical structures: comparison of geometric searching algorithms. *J Mol Graph* 5:49-56.

Brooks *et al.*, (1983) *J Comp Chem* 4:187-217.

Brünger AT (1992) X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR, Yale University Press, New Haven, Connecticut, United States of America.

20 Brünger AT, Adams PD, Clore GM, DeLano WL, Gros P, Grosse-Kunstleve RW, Jiang JS, Kuszewski J, Nilges M, Pannu NS, Read RJ, Rice LM, Simonson T & Warren GL (1998) Crystallography & Nmr System: A New Software Suite for Macromolecular Structure Determination, *Acta Crystallogr D Biol Crystallogr* 54:905-921.

25 Brzozowski *et al.* (1997) *Nature* 389:753.

Bugg CE, Carson WM & Montgomery JA (1993) Drugs by design. *Scientific Am* Dec:92-98.

Case *et al.*, AMBER 5, University of California, San Francisco, 1997.

30 Cohen NC, Blaney JM, Humblet C, Gund P & Barry DC (1990) Molecular Modeling Software and Methods for Medicinal Chemistry. *J Med Chem* 33:883-894.

-322-

Collaborative Computational Project, Number 4, (1994) *Acta Cryst.* D50, 760-63.

Connolly ML (1983) Solvent-Accessible Surfaces of Proteins and Nucleic Acids. *Science* 221:709-713.

- 5 Cowtan, (1994), *Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography*, 31, p 34-8

Creighton (1983) Proteins: Structures and Molecular Principles, W.H. Freeman & Co., New York, United States of America.

- 10 Cwirla SE, Peters EA, Barrett RW & Dower WJ (1990) Peptides on phage: a vast library of peptides for identifying ligands. *Proc Natl Acad Sci U S A*, 87:6378-6382.

Dauter Z, Li M & Wlodawer A (2001) Practical experience with the use of halides for phasing macromolecular structures: a powerful tool for structural genomics. *Acta Crystallog D Biol Crystallogr* 57::239-49.

- 15 DesJarlais RL, Sheridan RP, Dixon JS, Kuntz ID & Venkataraghavan R (1986) Docking flexible ligands to macromolecular receptors by molecular shape. *J. Med. Chem.* 29:2149-2153.

- 20 DesJarlais RL, Sheridan RP, Seibel GL, Dixon JS, Kuntz ID & Venkataraghavan R (1988) Using shape complementarity as an initial screen in designing ligands for a receptor binding site of known three-dimensional structure. *J. Med. Chem.* 31:722-729.

Devlin JJ, Panganiban LC & Devlin PE (1990) Random peptide libraries: a source of specific protein binding molecules. *Science*, 249:404-406.

- 25 Ducruix & Geige (1992) Crystallization of Nucleic Acids and Proteins: A Practical Approach, IRL Press, Oxford, England.

Dunbrack RL Jr., Gerloff D, Bower M, Chen X, Lichtarge O, & Cohen FE (1997). Meeting Review: The Second Meeting for the Critical Assessment of Protein Structure Prediction. *Folding & Design* 2:R27-R42.

- 30 Ebel S, Lane AN & Brown T (1992) Very stable mismatch duplexes: structural and thermodynamic studies on tandem G.A mismatches in DNA. *Biochem.* 31:12083-12086.

-323-

Eisen MB, Wiley DC, Karplus M & Hubbard RE (1994) Hook: A Program for Finding Novel Molecular Architectures That Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site. *Proteins* 19:199-221.

5 Erickson JW (1993) *Perspectives in Drug Discovery and Design* 1:109-128.

Fiser A, Do RK & Sali A (2000) Modeling of loops in protein structures. *Protein Sci* 9:1753-73.

10 Fitzgerald PMD (1988) MERLOT, an integrated package of computer programs for the determination of crystal structures by molecular replacement. *J Appl Cryst* 21:273-278.

Freedman LP (1999) Increasing the Complexity of Coactivation in Nuclear Receptor Signaling. *Cell* 97:5-8.

15 Goeddel DV (1990) Gene Expression Technology. Methods in Enzymology vol. 185, Academic Press, San Diego, California, United States of America.

Goodford PJ (1985) A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules. *J Med Chem* 28:849-857.

20 Goodsell DS & Olson AJ (1990) Automated Docking of Substrates to Proteins by Simulated Annealing. *Proteins* 8:195-202.

Goodwin B, Moore LB, Stoltz CM, McKee DD & Kliewer SA (2001) Regulation of the Human Cyp2b6 Gene by the Nuclear Pregnane X Receptor. *Mol Pharmacol* 60:427-431.

25 Greer J (1985) Model structure for the inflammatory protein C5a. *Science* 228:1055-1060.

Gribskov M & Burgess RR (1986) Sigma Factors from *E. coli*, *B. Subtilis*, Phage Sp01, and Phage T4 Are Homologous Proteins. *Nucleic Acids Res* 14:6745-6763.

30 Gronemeyer H & Laudet V (1995) Transcription Factors 3: Nuclear Receptors. *Protein Profile* 2:1173-1308.

-324-

- Gutberlet T, Heinemann U & Steiner M (2001) Protein crystallography with neutrons--status and perspectives. *Acta CrystallogrD Biol Crystallogr* 57:349-54.
- Handschin C, Podvinec M, Looser R, Amherd R & Meyer UA (2001) Multiple
5 Enhancer Units Mediate Drug Induction of Cyp2h1 by Xenobiotic-Sensing Orphan Nuclear Receptor Chicken Xenobiotic Receptor. *Mol Pharmacol* 60:681-689.
- Hauptman H (1997) Phasing Methods for Protein Crystallography. *Curr Opin Struct Biol* 7:672-680.
- 10 Hendrickson WA (2000) Synchrotron crystallography. *Trends Biochem Sci* 25:637-43.
- Hendrickson WA & Ogata CM (1997) Methods in Enzymology, Vol. 276, pp. 494-523, San Diego, California, United States of America.
- Honkakoski P, Zelko I, Sueyoshi T & Negishi M (1998) The Nuclear Orphan
15 Receptor Car-Retinoid X Receptor Heterodimer Activates the Phenobarbital-Responsive Enhancer Module of the Cyp2b Gene. *Mol Cell Biol* 18:5652-5658.
- Jakes *et al.* (1986) *J Mol Graph* 4:12-20.
- Jakes *et al.* (1987) *J Mol Graph* 5:41-48.
- 20 Jancarik J & Kim S-H (1991) Sparse matrix sampling: a screening method for crystallisation of proteins. *J Appl Cryst* 24:409-411.
- Jones TA, Zou J-Y, Cowan S & Kjeldgaard M (1991) Improved methods for building protein models into electron density maps and the location of errors in these models. *Acta Crystallogr A* 47:100-119.
- 25 Kahn R & Fourme R (1997) Methods in Enzymology, Vol. 276, pp. 268-286, Academic Press, San Diego, California, United States of America.
- Kastner P, Mark M & Chambon P (1995) Nonsteroid Nuclear Receptors: What Are Genetic Studies Telling Us About Their Role in Real Life? *Cell* 83:859-869.
- 30 Kawamoto T, Sueyoshi T, Zelko I, Moore R, Washburn K & Negishi M (1999) Phenobarbital-Responsive Nuclear Translocation of the Receptor Car in Induction of the Cyp2b Gene. *Mol Cell Biol* 19:6318-6322.

-325-

Kleywegt GJ & Brunger AT (1996) Checking your imagination: applications of the free R value. *Structure* 4:897-904.

Knighon DR, Pearson RB, Sowadski JM, Means AR, Ten Eyck LF, Taylor SS & Kemp BE (1992) Structural basis of the intrasteric regulation of myosin light chain kinases. *Science* 258:130-135.

Kuntz ID, Blaney JM, Oatley SJ, Langridge R & Ferrin TE (1982) A Geometric Approach to Macromolecule-Ligand Interactions. *J Mol Biol* 161:269-288.

Kyte J & Doolittle RF (1982) A Simple Method for Displaying the Hydropathic Character of a Protein. *J Mol Biol* 157:105-132.

Lam PYS, Jadhav PK, Eyermann CJ, Hodge CN, Ru Y, Bacheler LT, Meek JL, Otto MJ, Rayner MM, Wong YN, Chang C-H, Weber PC, Jackson DA, Sharpe TR & Erickson-Viitanen S (1994) Rational Design of Potent, Bioavailable, Nonpeptide Cyclic Ureas as HIV Protease Inhibitors. *Science* 263:380-384.

Lambert, (1997) in Practical Application of Computer-Aided Drug Design, (Charifson, ed.), pp. 243-303, Marcel-Dekker, New York

Lanz RB & Rusconi S (1994) A Conserved Carboxy-Terminal Subdomain Is Important for Ligand Interpretation and Transactivation by Nuclear Receptors. *Endocrinology* 135:2183-2195.

Laskowski RA, McArthur MW, Moss DS & Thornton JM (1993) PROCHECK: A program to check the stereochemical quality of protein structures. *J Appl Cryst* 26:283-291.

Lattman E (1985) Diffraction Methods for Biological Macromolecules. Use of the Rotation and Translation Functions. *Methods Enzymol* 115:55-77.

Lattman EE (1996) No crystals no grant. *Proteins* 25:i-ii.

Lawrence MC & Davis PC (1992) CLIX: a search algorithm for finding novel ligands capable of binding proteins of known three-dimensional structure. *Proteins* 12:31-41.

Levitt DG (2001) A new software routine that automates the fitting of protein X-ray crystallographic electron-density maps. *Acta Crystallogr D Biol Crystallogr* 57:1013-1019.

-326-

- Luthy R, Bowie JU & Eisenberg D (1992) Assessment of protein models with three-dimensional profiles. *Nature* 356:83-85.
- Mangelsdorf DJ & Evans RM (1995) The R α r Heterodimers and Orphan Receptors. *Cell* 83:841-850.
- 5 Martin YC (1992) 3d Database Searching in Drug Design. *J Med Chem* 35:2145-2154.
- McCree DM *et al.* (1992) *J. Mol. Graphics* 10:44-46.
- McKenna NJ & O'Malley BW (2000) From Ligand to Response: Generating Diversity in Nuclear Receptor Coregulator Function. *J Steroid Biochem*
- 10 *Mol Biol* 74:351-356.
- McPherson *et al.*, (1989) Preparation and Analysis of Protein Crystals, Robert E. Krieger Publishing Company, Malabar, Florida, United States of America.
- McPherson, *Eur J Biochem* 189:1-23, 1990.
- 15 McRee, *J Mol Graphics* 10: 44-47, 1992
- McRee, Practical Protein Crystallography, Academic Press, New York, 1993.
- Miller R, DeTitta GT, Jones R, Langs DA, Weeks CM & Hauptman HA (1993) On the Application of the Minimal Principle to Solve Unknown Structures. *Science* 259:1430.
- 20 Miranker A & Karplus M (1991) Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method. *Proteins* 11:29-34.
- Moore LB, Parks DJ, Jones SA, Bledsoe RK, Consler TG, Stimmel JB, Goodwin B, Liddle C, Blanchard SG, Willson TM, Collins JL & Klierer SA (2000) Orphan Nuclear Receptors Constitutive Androstane
- 25 Receptor and Pregnane X Receptor Share Xenobiotic and Steroid Ligands. *J Biol Chem* 275:15122-15127.
- Moras D & Gronemeyer H (1998) The Nuclear Receptor Ligand-binding Domain: Structure and Function. *Curr Opin Cell Biol* 10:384-391.
- Murshudov GN, Vagin AA, Lebedev A, Wilson KS & Dodson EJ (1999)
- 30 Efficient anisotropic refinement of macromolecular structures using FFT. *Acta Cryst D Biol Crystallogr* 55:247-255.

-327-

Navaza, (1994) AMoRe: an automated package for molecular replacement, *Acta. Cryst. A*50: 157-163

Navia MA & Murcko MA (1992) Use of structural information in drug design *Curr Opin Struct Biol* 2:202-210.

- 5 Needleman SB & Wunsch CD (1970) A General Method Applicable to the Search for Similarities in the Amino Acid Sequence of Two Proteins. *J Mol Biol* 48:443-453.

- Nicholls A, Sharp KA & Honig B (1991) Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. *Proteins* 11:281-96.

10 Nishibata & Itai, (1991) *Tetrahedron* 47:8985-8990.

- Nolte RT, Wisely GB, Westin S, Cobb JE, Lambert MH, Kurokawa R, Rosenfeld MG, Willson TM, Glass CK & Milburn MV (1998) Ligand-binding and Co-Activator Assembly of the Peroxisome Proliferator-Activated Receptor-Gamma. *Nature* 395:137-143.

Otwinowski (1993) in Proceedings of the CCP4 Study Weekend: Data Collection and Processing. Sawyer *et al.*, eds., pp.56-62, SERC Daresbury Laboratory, England.

- Paech K, Webb P, Kuiper GGJM, Nilsson S, Gustafsson J-A, Kushner PJ & Scanlan TS (1997) Differential Ligand Activation of Estrogen Receptors ER α and ER at Ap1 Sites. *Science* 277:1508-1510.

- 20 Parks DJ, Blanchard SG, Bledsoe RK, Chandra G, Consler TG, Kliewer SA, Stimmel JB, Willson TM, Zavacki AM, Moore DD & Lehmann JM (1999) Bile Acids: Natural Ligands for an Orphan Nuclear Receptor. *Science* 284:1365-1368.

25 Pearlman *et al.*, (1995) AMBER, a package of computer programs for applying molecular mechanics, a normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules *Comput. Phys. Commun.* 91: 1-41.

- 30 Perrakis A, Morris R & Lamzin VS (1999) Automated protein model building combined with iterative structure refinement. *Nature Structural Biology* 6:458-463.

-328-

Petsko GA (1985) Methods in Enzymology, Vol. 114, pp. 147-156, Academic Press, Orlando, Florida, United States of America.

Rarey *et al.*, *J Comput Aid Mol Des*, 10:41-54, 1996.

Rossmann, ed, (1972) The Molecular Replacement Method, Gordon & Breach, New York, New York, United States of America.

Sambrook J & Russell DW (2001) Molecular Cloning : A Laboratory Manual, 3rd ed. Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York, United States of America.

Schulz GE & Schirmer RH (1979) Principles of Protein Structure, Springer-Verlag, New York, New York, United States of America.

Schwartz *et al.*, eds., (1979), Atlas of Protein Sequence and Structure, National Biomedical Research Foundation, pp. 357-358.

Scott JK & Smith GP (1990) Searching for Peptide Ligands with an Epitope Library. *Science* 249:386-390.

Sheldrick, *Acta Cryst*, A46: 467, 1990.

Shiau *et al.*, (1998) *Cell* 95:927.

Smith TF & Waterman M (1981) Comparison of Biosequences. *Adv Appl Math* 2:482-489.

Stein B, Yang MX. Repression of the interleukin-6 promoter by estrogen receptor is mediated by NF-kB and C/EBP beta. *Mol. Cell. Biol.* 15, 4971-4979 (1995).

Stoddard BL (1998) New results using Laue diffraction and time-resolved crystallography. *Curr Opin Struct Biol* 8:612-8.

Tibanyenda N, De Bruin SH, Haasnoot CA, van der Marel GA, van Boom JH & Hilbers CW (1984) The effect of single base-pair mismatches on the duplex stability of d(T-A-T-T-A-A-T-A-T-C-A-A-G-T-T-G) . d(C-A-A-C-T-T-G-A-T-A-T-T-A-A-T-A). *Eur J Biochem* 139:19-27.

Tijssen P (1993) Overview of principles of hybridization and the strategy of nucleic acid probe assays in Laboratory Techniques in Biochemistry and Molecular Biology-Hybridization With Nucleic Acid Probes., Elsevier, New York, New York, United States of America.

Tora *et al.*, (1988) *Nature* 333: 677-684.

-329-

- Tosatto SC, Bindewald E, Hesser J & Manner R. (2002) A divide and conquer approach to fast loop modeling, *Protein Eng* 15:279-86.
- Tsai and O'Malley, (1994) Molecular mechanisms of action of steroid/thyroid receptor superfamily members, *Ann. Rev. Biochem.* 63: 451-486
- 5 Tzukerman MT, Esty A, Santiso-Mere D, Danielian P, Parker MG, Stein RB, Pike JW & McDonnell DP (1994) Human Estrogen Receptor Transactivational Capacity Is Determined by Both Cellular and Promoter Context and Mediated by Two Functionally Distinct Intramolecular Regions. *Mol Endocrinol* 8:21-30.
- 10 Villieux FMD & Read RJ (1997) Methods in Enzymology, Vol. 277, pp. 18-52, Academic Press, Orlando, Florida, United States of America.
- Waxman DJ (1999) P450 Gene Induction by Structurally Diverse Xenochemicals: Central Role of Nuclear Receptors Car, Pxr, and Ppar. *Arch Biochem Biophys* 369:11-23.
- 15 Weatherman RV, Fletterick RJ & Scanlan TS (1999) Nuclear-Receptor Ligands and Ligand-binding Domains. *Annu Rev Biochem* 68:559-581.
- Weber PC (1991) Physical Principles of Protein Crystallization. *Adv Protein Chem* 41:1-36.
- Weeks CM, DeTitta GT, Hauptman HA, Thuman P & Miller R (1994) Structure
20 solution by minimal-function phase refinement and Fourier filtering. II. Implementation and applications. *Acta Crystallogr A* 50:210-20.
- Wellner, (1971) *Anal. Chem.* 43:597.
- West ML, Fairlie DP (1995) Targeting HIV-1 protease: a test of drug-design methodologies. *Trends Pharmacol Sci* 16:67-74.
- 25 Westbrook EM & Naday I (1997) Methods in Enzymology, Vol. 276, pp. 244-268, Academic Press, San Diego, California, United States of America.
- Wlodawer A & Erickson JW (1993) Structure-based inhibitors of HIV-1 protease. *Ann Rev Biochem* 62:543-585.
- Xiao, Li, Xiaoming, Cui, Madison, Vincent, White, Ronald E, and Cheng, K-C,
30 (2002) Insights from a three-dimensional model into ligand-binding to Constitutive Active Receptor, *Drug Metabolism and Disposition* 30:951-956.

-330-

Xie W, Barwick JL, Simon CM, Pierce AM, Safe S, Blumberg B, Guzelian PS & Evans RM (2000a) Reciprocal Activation of Xenobiotic Response Genes by Nuclear Receptors Sxr/Pxr and Car. *Genes Dev* 14:3014-3023.

- 5 Xie W, Barwick JL, Downes M, Blumberg B, Simon CM, Nelson MC, Neuschwander-Tetri BA, Brunt EM, Guzelian PS & Evans RM (2000b) Humanized Xenobiotic Response in Mice Expressing Nuclear Receptor Sxr. *Nature* 406:435-439.

- Zhang KYJ, Cowtan K & Main P (1997) Methods in Enzymology, Vol. 277, pp.
10 53-64, Academic Press, Orlando, Florida, United States of America.

U.S. Patent No. 4,554,101

U.S. Patent No. 6,008,033

- 15 It will be understood that various details of the invention can be changed without departing from the scope of the invention. Furthermore, the foregoing description is for the purpose of illustration only, and not for the purpose of limitation, the invention being defined by the claims.